HIGH FIELD QUANTUM TRANSPORT THEORY

IN SEMICONDUCTORS

by

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A thesis

presented to the University of Warwick

in partial fulfillment of the requirements

for entry to the degree of

Doctor of Philosophy

Department of Physics

June 1983

Abstract

A technique based on the Wigner distribution phase space interpretation of quantum mechanics is developed to obtain a transport theory capable of describing the high-field, inhomogeneous electronic transport in collision dominated sub-micron semiconductor devices.

The problems associated with the general construction of quantum phase space distributions are considered using the Marcinkiewicz theorem which suggests that any defined quantum distribution which is both real and bounded must also, in general, be allowed to assume negative values.

A pair of exact coupled transport equations for the one-electron and one-phonon Wigner distribution functions is obtained using multiple imaginary time Greens function techniques starting from a model Hamiltonian incorporating electron-electron and electron-phonon interactions as well as a coupling to externally applied space-and time-dependent electric and pressure fields. These exact equations exhibit a non-locality which may be interpreted in terms of the uncertainty relations of quantum mechanics.

Assumptions are made (the many body correlation effects being approximated using functional derivative techniques) which restrict the resulting equations to the transition regime between the bulk scale device adequately modelled by Boltzmann transport and the microscopic region driven exclusively by boundary influences. These approximate equations maintain a non-locality due to the finite extent of a collision process thus allowing the collision integrals to become explicitly dependent on the driving field. Derived self-consistently within the collision integrals is a dynamical non-equilibrium screening of the interaction potentials which is also explicitly field-dependent.

The field-dependence of the effective interactions is analysed for several model screening functions in two-and three-dimensional electron assemblies for a range of system parameters in GaAs. The results indicate that conventional screening overestimates the efficiency of the shielding process and that the action of a strong field within a collision event descreens the effective interaction potentials.

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Acknowledgements

There are many who have assisted, in one form or another, in the completion of this work, a few of whom I would now like to thank.

First to Doctor John R. Barker for providing just the correct balance of motivation and optimisim that the production of this thesis required.

Secondly, to the Department of Physics, and in particular to the staff of the theoretical physics section for providing a suitable environment in which I was able to develop an interest in the dynamical approach to physics. I would also like to acknowledge the use of the Department's synergetics group's computer, an HP 9845C, which generated all the diagrams in this thesis.

As for the excellent typing, the credit belongs to Nada Gvero who's cheerfulness made the final preparation of this thesis far less of an ordeal than was anticipated.

Finally, I gratefully acknowledge the financial support provided by the Science and Engineering Research Council.

Declaration

This thesis contains an account of my own independent research work performed in the Department of Physics at the University of Warwick between October, 1979 and October, 1982 under the general supervision of Doctor John R. Barker.

Certain aspects of this work have already been exposed to the scientific literature in the form of joint publications, as follows:-

1. "Quantum theory of hot electron-phonon transport in inhomogeneous semiconductors", J. R. Barker and D. Lowe, J. de Physique, Coll. C7, suppl. au no. 10 Tome 42, C7-293 (1981).

2. "A Wigner function approach to transport and switching in sub-micron heterostructures", J. R. Barker, D. Lowe and S. Murray in "Physics of sub-micron devices", edited by D. K. Ferry and K. Hess. (Plenum Press, New York, 1982)(in the press).

3. "Quantum theory of field-dependent shielding of scattering interactions in semiconductors", D. Lowe and J. R. Barker, an oral presentation at the 2nd Annual General Conference of the Condensed Matter Division of the European Physical Society, March, 1982.

To my daughters

CHAPTER 1

GENERAL INTRODUCTION

§1.1. Motivation for the thesis

Perhaps the single most important influence on society in the last quarter of a century has been the advent of the transistor and the subsequent evolution of the integrated circuit as a rapid information processing unit. Due to the requirements of more efficient and complex logic systems it has been found necessary to produce faster operating individual devices by essentially making them smaller using progressively more sophisticated and expensive fabrication techniques.

Consequently it is pertinent to enquire just how small it is possible to make a device that acts in a physically predictable way, since it has previously been pointed out[12] that this downscaling principle is restricted by fundamental limitations imposed by extrapolating our bulk scale knowledge down to the microscopic level. The argument may be summarised thus.

Our understanding of the operation of contemporary devices is based on semiclassical concepts extracted essentially from the Boltzmann transport equation; a theory originally developed for classical dilute gases and extended to the gas-like quasi-particle excitations in condensed matter. That this theory has given such excellent results in problems far removed from its' original range of validity is a testimonial to an element of fundamental correctness that must be contained within its' derivation. However there are features explicit in its' construction that limit its' strict validity to what might be termed the bulk scale device, which are primarily due to its' treatment of collisions which are considered instantaneous, point-like and structureless. That is to say the Boltzmann equation describes the free accelerative transport of particles

in effective driving fields being randomly interrupted by sudden, disruptive and irreversible scattering events into different accelerative modes: the collisions have no other role than providing a randomisation mechanism that constitutes a continuous loss of information from the system.

However, since collisions are not point-like (the extent being characterised by a Debye screening length for example in the case of a hot Maxwellian plasma) we see that the Boltzmann transport equation assumes that the distance between collisions (L_f) is much greater than the extent of a collision (L_c). Moreover since the electrons in the colliding region are taken to have an infinite lifetime (negligible boundary effects) an accompanying assumption is that the characteristic device scale (L - the channel length for instance) is much greater than the mean separation between collisions. Thus Boltzmann transport theory applies to situations that enjoy the spatial separation criterion:

$$L > L_f >> L_c \qquad (1.1.1.).$$

Unfortunately it is a consequence of small devices that high electron densities are required and typically in the range of $10^{16} - 10^{17}$ cm^{-3}[42]. Consequently since the range of a collision must inevitably remain finite (due to the long range of the Coulomb interaction) as the density of carriers increases the mean duration of a collision will become of the same order of magnitude as the time spent travelling between collisions. In this case we would have an inequality of the form

$$L > L_f \approx L_c \qquad (1.1.2.)$$

where the Boltzmann equation is incapable of predicting the correct behaviour due to its' naive treatment of collisions.

Furthermore in the extreme technological limit of small devices the very small active channel region would mean that the extent of a collision would constitute an appreciable fraction of the characteristic device size. In such a situation the concept of a mean distance between collisions would become meaningless and such devices would conform to the criterion

$$L \simeq L_c \qquad (1.1.3.).$$

Current devices are being built on the 1-2 micron scale where it is already appreciated that the Boltzmann transport theory has limited usefulness[71]. Therefore in order to consider the physics of devices characterised by the spatial criteria (1.1.2.) and (1.1.3.) Barker and Ferry[12] have found it convenient to introduce two archetypal devices based on the MOS transistor called the medium-and very-small-device.

Within this scheme a bulk scale device is defined for typical sizes down to about 2500 Å where the semiclassical Boltzmann equation is considered a reasonable representation of the physics involved. The medium-small-device is conjectured to have active regions in the spatial range of 250 to 2500 Å where the criterion (1.1.2.) is considered to hold. Consequently, although many collisions still occur across a channel length, the finite extent of each collision means that the electron evolution across the channel is governed by the dynamics that occur actually within the scattering event - a general behaviour beyond the scope of the Boltzmann equation. Below 250 Å is the regime of the very-small-device characterised by criterion (1.1.3.) which is not so much influenced by the (very few) collisions in the channel but by the potentials of the device boundaries.

Neither the medium-nor very-small-device is capable of being described by any current transport theory and in particular semiclassical Boltzmann theory. Therefore as fabrication methods push well into the

submicron regime we are unable to adequately model the physics involved. We might anticipate that the medium-small-device would be amenable to a Boltzmann-like transport equation but with a modified collision integral to make allowances for the dynamic behaviour within a collision process, but we would certainly require a complete quantum dynamical transport theory to model the very-small-device.

The situation is further complicated because the transport in submicron devices must evolve under very strong electric fields. This is because the scaling principle eventually fails when applied to the switching field because the transfer of information is a thermodynamically irreversible process requiring an energy of at least $k_B T$ and more typically 10-100 $k_B T$ in order to reduce noise fluctuation. Consequently as an order of magnitude estimate, the electric field required to irreversibly switch across a channel length of one micron supplying an energy of 10 $k_B T$ at T = 300 K is 2.5 kV cm^{-1}.

Therefore below the one micron threshhold we are faced with the problem of attempting to model extremely non-equilibrium quantum transport in very strong electric fields. In the authors opinion there does not yet exist a consistent descriptive framework for a transport theory from which realistic numerical simulations may be constructed to describe these future conjectured devices. It is primarily this lack of a coherent method that has provided the motivation for this thesis.

§1.2. Scope

Bearing in mind the motivation of this study the underlying theme of the thesis is the construction of a suitably complex and yet convenient framework capable of modelling high field quantum transport in submicron devices. In particular the emphasis is placed on an adequate description of the transition regime between the semiclassical bulk device and the fully quantum dynamical case of the very-small-device. Thus the situation

with which we are primarily concerned corresponds to the medium-small-device defined in the typical spatial range of 250-2500 Å where the many body effects of collisions in strong electric fields have a controlling influence.

The transport theory is developed in a quantum mechanical phase-space analogous to the classical phase-space inherent in the Boltzmann equation. This is because the usual interpretation of quantum mechanics is neither mathematically nor conceptually simple and particularly when applied to the many body problem but also, because of the success of the Boltzmann equation, we would hope that a phase-space formulation of quantum transport would allow some of the methods developed for problems in semiclassical theory to be adaptable enough to apply to quantum dynamical transport through an appropriate phase-space transport equation. At the very least a phase-space formulation should allow a critical comparison between the structures of quantum and classical dynamics being compared in the same space but using different algebras[17].

Because the phase-space approach to quantum mechanics is not generally a familiar subject, a few associated problems with its' construction will be discussed by the use of a mathematical theorem due to Marcinkiewicz[62], the consequences of which will be seen to constitute a good argument against the general use of truncation schemes in many body theory.

The particular quantum phase-space density used in this thesis is the one first introduced by Wigner[97] in terms of which it is possible to obtain reasonable transport equations for the Wigner one-electron and one-phonon phase-space distribution functions under a model Hamiltonian including the effects of electron-electron and electron-phonon interactions in externally applied electric and pressure fields. The approximation techniques used are non-perturbative in the sense that they do not depend on the absolute magnitudes of the fields nor

of the interactions and consequently the resulting transport equations are valid for strong electric fields.

However a certain class of approximations is assumed which restricts the theory to the medium-small-device but it will be further discussed how these restrictions may be relaxed to allow a description of the very-small-device in terms of quantum ballistic transport.

The particular results of this approach exhibit that the transport collision integrals are explicitly dependent on the effective field driving the system (entirely due to the field being allowed to act within a collision event), an effect independently noted by Levinson[57] and Barker[8] and denoted by the latter the intracollisional-field-effect.

This intra-collisional-field-effect is manifest in two ways: first it distorts the energy conservation factors, thus inducing threshhold lowering of emission processes for example, and secondly it modifies the collision process itself by altering the dynamics of the electron-electron screening interaction. The latter modification has received little or no attention whatsoever in the published literature, a deficiency redressed in this thesis when the effect of a strong field is considered on various model screening functions where it is seen to affect the interactions considerably.

It should be stressed however that such results are only tentative being based on a theory built for a projected need and as such there are no experiments to compare directly with yet. However there are already special circumstances (refering here in particular certain aspects of Dingle devices[24]) where the semiclassical approach to transport should be stretched beyond its' limit. In such cases theory and experiment should disagree quantitively if not qualitatively no matter how carefully the theoretical calculations are performed. This would provide an initial testing area where a modified transport theory could suggest corrections beyond the scope of the conventional theory.

In short, then, the thesis offers a predictive quantum dynamical phase-space transport theory in strong electric fields applicable to collision dominated transport in submicron semiconductor devices where a novel modification to the dynamics, the interaction-field-effect, is considered explicitly.

§1.3. Survey of chapters

This thesis considers the high field quantum transport problem in three distinct and related areas which may broadly be categorised as (a) elucidating the problems; (b) constructing a transport theory; and (c) explicitly calculating unique features. These areas have been subdivided into the following chapters.

Chapter 2 takes three typical current approaches used to study high field transport which have been termed the Boltzmann equation, the wavefunction and the equation-of-motion techniques respectively. Each is briefly considered and their respective features and advantages are noted.

Chapter 3 is also in the category of elucidating problems although the difficulties here are more of a technical nature. Essentially the chapter is concerned with the proof and consequences of the Marcinkiewicz theorem in terms of the characteristic (or moment-generating) function of distributions. It is seen that the theorem imposes strict limitations regarding the use of truncation methods in many body theory where it is assumed reasonable to neglect the n-th order and higher moments for some large n which is typically taken to be of order three. The theorem also has a use in the construction of general quantum phase-space distribution functions since it illustrates that if the distribution is so defined as to be real and bounded (in the sense that its' integral is finite) then it must generally be allowed to assume negative values somewhere in its' range of definition thus invalidating it of a strict interpretation as a

probability density (as for example afforded by the classical distribution function). The choice of a quantum distribution is not unique but the Wigner distribution used in this thesis is explicitly constructed in Chapter 3 in terms of the density matrix. It is also shown how to associate the Wigner equivalent of an observable represented by an Hermitian operator with a real phase-space function so that expectation values may be calculated as integrations over the phase-space co-ordinates analogous to the usual classical procedure.

Chapter 4 provides the meat of the thesis since it develops the transport theory by obtaining coupled equations of motion for electron and phonon Wigner distributions. By necessity it is of a mathematically rigorous nature interspersed with the relevant physical approximations. The techniques used rely heavily on multiple imaginary time Greens functions where the many body correlations are introduced and approximated using functional derivative techniques. The Wigner distributions are obtained from corresponding Greens functions using a series of formal identities and consistency relations. The model assumed in this chapter takes an interacting system of electrons with electrons and electrons with non-polar phonons all subjected to externally applied space-and time-dependent classical electric and pressure fields driving the electrons and phonons respectively. The self consistent calculations yield amongst other details, an explicitly field dependent, non-equilibrium screening function that dynamically shields the interactions.

Chapter 5 considers this screening function (which has a Lindhardt-like structure[39]) in some detail. Various approximate forms are obtained using several model distribution functions for both two-and three-dimensional electron plasmas using parameters appropriate to GaAs where necessary. The dependence of these model forms is analysed both analytically and numerically as the electron density and temperature

is changed and, most important of all, as the (strong) electric field is varied.

Chapter 6 summarises the results of the thesis which are discussed with regard to the expected modifications in these small devices due to the dynamic behaviour of the collisions. Amongst the future areas of research suggested by the thesis also discussed in this Chapter, is an illustration of how the theory may be extended to describe the fully quantum ballistic transport expected in the very-small-device.

The appendices contain material either of a background nature to be used in conjunction with the relevant chapters, mathematical calculations only the results of which are considered important, or original results directly generated from the thesis although not particularly relevant to the central theme.

CHAPTER 2

CRITICAL REVIEW OF CURRENT METHODS APPLIED TO MODEL QUANTUM TRANSPORT IN SUBMICRON DEVICES

The philosophies of existing quantum transport theories range through the entire spectrum bounded by the phenomenological and the purely formal. Consequently this chapter is limited to an analysis of three representative theories in common current usage which, in ascending order of mathematical complexity are: the Boltzmann equation approach, a wave function technique and finally a kinetic equation of motion method. These three basic theories have been singled out for attention because between them they embody the characteristics and difficulties of almost all transport theories to date. Common to most theories though is the assumption of the existence of a phase-space distribution function f(R,P,T) to be obtained from its corresponding equation of motion, where the problem faced by transport theorists is to obtain an explicit form for this equation. The first such theory considered is representative of the phenomenological approach to transport and is the Boltzmann equation method.

§2.1. The Boltzmann Equation approach

This scheme borrows heavily from the classical transport theory based on the equation introduced a century ago by Boltzmann. To make allowances for quantum mechanical behaviour, the distribution function has to be assumed to be coarse-grained in some way to allow the distribution function to describe the simultaneous measurement of position and momentum; the electron velocity v is related to the Bloch momentum $p = \hbar k = mv$ and allowances for quantum processes in collision events have to be convolved within the scattering rate W(p'p) from a momentum state p' to p. Bearing these points in mind it seems obvious how to

write down the equation of motion for the distribution function, specifically

$$[\partial_t + v\cdot\partial_r + eE\cdot\partial_{\underline{p}}]f(r,p,t) = \sum_{p'} \{W(p',p)f(p'rt) - W(p,p')f(p,r,t)\} \qquad (2.1.1.)$$

The collision integrals in (2.1.1.) are usually obtained by a Fermi Golden rule procedure so that the scattering rates are proportional to the final density of states and the squared interaction matrix elements $\tilde{V}(p)$, i.e.

$$W(p',p) \propto |\tilde{V}(p' - p)|^2 \delta[\varepsilon(p) - \varepsilon(p') \pm \hbar\omega_{p'-p}] \qquad (2.1.2.)$$

in the case of energy conservation. The δ-function appearing in (2.1.2.) represents the precise energy conservation between the scattered electron momentum state p' to p and a colliding body carrying the excess energy $\hbar\omega_{p'-p}$ away from the collision.

There are several comments we may immediately infer from the implications of this framework: the effective driving field E (which should correctly be determined in a self consistent fashion by coupling with Poisson's equation) and the inter-particle collisions are treated as separate independent perturbations to the otherwise free motion; the collisions themselves are considered as point events so that the effects of one collision may be considered in isolation to subsequent collisions (note that the precise form of energy conservation requires an infinite amount of time after the collision to be established before undergoing another collision) and consequently the electric field can play no role in determining the dynamics of a single collision process.

Considering the basis of the Boltzmann-Bloch equation (2.1.1.) it has had remarkable success in describing the behaviour of the large-scale semiconductor device by the use of numerical Monte Carlo[28] and iterative[76] solutions of specific examples of (2.1.1.). Various approximate analytical solutions to the equation have been proposed,

most of which are based on the displaced Maxwellian distribution function (see Ferry p.117 in reference [71]).

$$f = A\exp[-(E - p\cdot v_d)/k_B T_e] \qquad (2.1.3.)$$

which is only specified by choosing the parameters A, v_d, T_e which have the significance, respectively, of a normalisation, a drift velocity the magnitude of which determines the shift of the peak of the function away from the origin and an effective electron temperature which determines how dispersed the distribution is.

The simple form of (2.1.3.) is due to a theorem of Fröhlich and Paranjape[34] based on the Boltzmann equation whereby if the electron concentration is sufficiently large then the isotropic part of the distribution function should be of a displaced Maxwellian form since the energy gained from the field may be quickly redistributed by all inter-particle collisions. Thus the electron distribution at a given instant may be considered to be in a quasi-internal equilibrium but with an effective temperature T_e (usually much greater than that of the surrounding lattice, hence the term "hot electrons") and an average momentum value of $m\, v_d$.

In this approach the transport theory is complete once the governing parameters A, v_d, T_e have been determined and these may be calculated from the first three moments of the Boltzmann equation (2.1.1.) since

$$\left.\begin{aligned} n &= \langle 1\rangle \\ m\, v_d &= \langle p\rangle \\ 3mk_B T_e &= \langle p^2\rangle \end{aligned}\right\} \qquad (2.1.4.)$$

where $\langle\phi(p)\rangle \equiv \int dp\,\phi(p) f(r,p,t)$ are the moments of the Boltzmann equation determined by the equations

$$\partial_t\langle\phi(p)\rangle + \partial_r\langle\phi(p)p/m\rangle + \langle eE\cdot\partial_p\phi(p)\rangle =$$

$$= \langle\sum_{p'}[\phi(p') - \phi(p)]W(p,p')\rangle \qquad (2.1.5.)$$

Thus substituting $\phi = 1, p, p^2$ respectively in (2.1.5.) will give us three coupled equations which may be self-consistently solved numerically provided the scattering terms are sufficiently simple and provided we neglect moments of p^3 and higher (we will return to this truncation procedure in §2.3.).

The result is a technique which has given tremendous insight into the physics of hot electron transport in large scale devices which has then been used to try and extrapolate into the realm of the medium-small device. However the credibility of this method has been called into question for a variety of reasons (although it is still used to study high field quantum transport: a recent example[46] is the use of (2.1.3.) to analyse electron-electron screening effects in submicron scale GaAs structures where the electric fields considered were up to 10 kV cm^{-1}).

The condition requiring a sufficiently large density of electrons greater than some critical concentration is often violated (see Hearn p.153 in reference [71]; also [14]) and consequently the electron assembly is unable to redistribute the energy acquired from the electric field particularly in certain non-equilibrium steady state situations such as the laser excitation of carriers into the conduction band[14]. Moreover we would not expect submicron devices to allow a pulse of electrons enough time to settle into a stationary state, albeit a non-equilibrium one, as is implicit in (2.1.3.) but would be determined entirely by the short time response to a suddenly applied field. There is also the criticism of neglecting the third and higher order moments, a fault it has in common with the equation of motion technique (§2.3.), the consequences of which will be considered in the next chapter.

The criticisms though are not limited to the approximate solution (2.1.3.) but may be extended to the original Boltzmann equation (2.1.1.). We have noted that the collisions as determined by Fermi's Golden rule are considered point-like and asymptotic: a carrier in a well defined non accelerating momentum state approaches the scatterer from the distant past, interacts and then passes into the distant future into another well defined stationary state. The Golden rule collapses this sequence of events into an instant and adds up the effects of all such instants.

Such a drastic reduction is not considered disastrous when the size of the system is macroscopic compared to the size of a collision event (as measured by the Debye screening length for example). However in submicron systems the extent and duration of a collision may constitute an appreciable fraction of the characteristic device lengths and times[12], in which case the instantaneous nature of collisions is lost. The sharp energy conservation factor explicit in (2.1.2.) is lost and the possibility arises for the electric field to contribute within a collision process thus blurring the distinction between driving field and scattering terms as separate perturbations.

Therefore we must conclude that although the Boltzmann equation approach has proved invaluable in providing us with a physical intuition with regard to electron transport in high electric fields, its' phenomenological form is incapable of incorporating certain effects due to the dynamic and non-local nature we would expect in sub-micron transport. The next section illustrates an attempt to incorporate electric field effects into the collision integral.

§2.2. The Wave Function Approach

The second popular scheme used to study high field quantum transport is based on a perturbative solution of Schrödinger's equation for the

electron wavefunction in some given convenient representation. The perturbation refered to here applies not to the electric field but to an assumed small particle-particle interaction which has the significance of effecting transitions between the complete set of states specified by the perturbationless wavefunctions.

Thus we take a Hamiltonian $H = H_o + V$ where we know the wavefunctions corresponding to H_o (which includes the applied electric field) and use this complete set to describe properties of the extended Hamiltonian. In particular we are concerned with the transition rate of scattering $R_{k,k'}$ from a momentum state $\hbar k$ to one of $\hbar k'$ which arises in the following manner.

We assume that at $t = 0$ the system is in a state $|\psi_n^o(t)>$ which is a solution of the Schrödinger equation corresponding to H_o. At a later time due to the perturbation V, the system is in a state $|\psi>$ which may be considered as a superposition of all the wavefunctions $\{\psi_n^o(t)\}$ suitably weighted by a factor $a_n(t)$, i.e.

$$|\psi> = \sum_n a_n(t)\,|\psi_n^o> \qquad (2.2.1.)$$

which obeys the equation

$$i\hbar\partial_t|\psi> = (H_o + V)\,|\psi> \qquad (2.2.2.)$$

Consequently the weighting factors must satisfy

$$i\hbar\partial_t a_m(t) = \sum_n a_n(t)<\psi_m^o|V|\psi_n^o> \qquad (2.2.3.)$$

subject to the boundary condition $a_m(0) = \delta_{n,m}$.

The assumption in first order perturbation theory is that $a_m(t)$ evolves only from $a_m(0)$, i.e. the assumption is that $a_n(t) = \delta_{n,m}$. Using this in (2.2.3.) gives an explicit expression for the weighting factors

$$a_n(t) = -\frac{i}{\hbar}\int_0^t d\tau \langle\psi_m^o(\tau)|V(\tau)|\psi_n^o(\tau)\rangle \qquad (2.2.4.)$$

Therefore from (2.2.1.) the probability P(t) that the system is in an eigenstate $|\psi_{n'}^o\rangle$ at a later time t, given that it was in the state $|\psi_n^o\rangle$ at t = 0 is just

$$P(t) \equiv |\langle\psi_{n'}^o|\psi\rangle|^2 = |a_{n'}(t)|^2 \qquad (2.2.5.)$$

with $a_{n'}$ given in (2.2.4.). In which case the rate of scattering between states n and n' may be defined as

$$R_{n,n'}(t) \equiv d_t P(t) = \frac{1}{\hbar^2} d_t \left|\int_0^t d\tau \langle\psi_{n'}^o(\tau)|V(\tau)|\psi_n^o(\tau)\rangle\right|^2 \qquad (2.2.6.)$$

Before we proceed to calculate this transition rate in a specific case there are a number of comments we should make.

This approach relies on the system being in an initially prepared eigenstate and scattering into another eigenstate which must be known in order to calculate transition rates. Unfortunately real submicron systems will never be in simple eigenstates and the Hamiltonian will be sufficiently complex (for example by the introduction of the electron-electron interaction) to render the extraction of eigensolutions impossible. We can also recognise an element of arbitrariness in this approach for a couple of reasons. The selection of an unperturbed and a perturbing part to the Hamiltonian involves an a priori knowledge of the dynamics described by this Hamiltonian whereas we shall see in Chapters 4 and 5 that the electron-phonon interaction for example, which is usually screened by the electron-electron interaction depends on the (large) electric field itself and so it is not obvious that such a simple division exists where the perturbation may be considered to be small. The second element of arbitrariness enters this approach through the definition of a transition rate (2.2.6.). In this Chapter we take it to be the time rate of change of the probability of a

transition between two states but alternative definitions exist. For example recently Herbert and Till[40][41] used the definition of the probability of a transition per unit time:-

$$R'_{nn'} = P(t)/t \qquad (2.2.7.)$$

to calculate the total scattering rate of Bloch electrons in a constant electric field off phonons. They obtained results which were in disagreement with the earlier works of Barker[9][10] and Thornber[91] and not surprisingly since the two definitions (2.2.7.) and (2.2.6.) are only equivalent in special circumstances (such as when the probability of a transition increases linearly with time which can only be true for short time scales. Since conventional scattering rates are then obtained by letting $t \to \infty$ the contradiction is obvious).

At this stage we have no criteria for deciding which, if either of the two definitions, is the correct one to use but must await a more complete transport theory (Chapter IV). Consequently we prefer to use (2.2.6.) in this section although the subsequent criticisms would apply equally well if we had used the alternative form (2.2.7.).

Leaving these general problems aside, the specific application of the method has its' own peculiar difficulties associated with the choice of an electromagnetic gauge which has given rise to a certain amount of confusion in the literature. It is to this problem we now address ourselves by illustration of the following model situation.

The unperturbed part of the Hamiltonian is taken as a free electron assembly which at a time $t = 0$ is subjected to a uniform though possibly time dependent electric field. This is perhaps the most complicated situation that may be handled by the wavefunction approach and certainly the most common[40][41][48][49][73][82]. Since the difficulties encountered in this model are of a technical rather than an interpretational nature it is necessary to consider the math-

ematical basis of this model in some detail.

The usual starting point is the Hamiltonian

$$H = \frac{1}{2m_i} \sum_i (P_i - \frac{e_i}{c} A(r_i,t))^2 + \sum_i e_i \phi(r_i,t) \qquad (2.2.8.)$$

where P_i is the canonical momentum to r_i which obey the commutation relations:

$$[P_x,x] = \hbar/i \ , \ [P_x,P_y] = 0 \qquad (2.2.9.)$$

and the electric (E) and magnetic (B) fields are expressed in terms of the scalar (ϕ) and vector (A) potentials by

$$\left.\begin{aligned} B &= \nabla \times A \\ \text{and} \quad E &= -\frac{1}{c} \partial_t A - \nabla\phi \end{aligned}\right\} \qquad (2.2.10.)$$

It is interesting to recall the origin of (2.2.8.) which derives from the Lagrangian[81]

$$L = \frac{1}{2} \sum_i m v_i^2 + \int \frac{d^3r}{8\pi} [E^2 - B^2] - \sum_i e_i \phi(r_i,t) + \\ + \sum_i \frac{e_i}{c} v_i \cdot A(r_i t) \qquad (2.2.11.)$$

chosen to generate Maxwells source equations as well as the classical equation of motion of a particle with charge e_i at r_i moving with velocity v_i in an electromagnetic field.

This Lagrangian is a function of three variables $\eta \epsilon [\phi,A,r]$ and their canonical momenta $P_\eta \equiv \partial L/\partial \dot{\eta}$ in terms of which the general Hamiltonian may be generated from the definition[36] $H \equiv \sum_i \dot{\eta}_i P_\eta - L$ to yield explicitly

$$H = \frac{1}{2m} \sum_i [P_i - \frac{e_i}{c} A(r_i,t)]^2 + \sum_i e_i \phi(r_i,t) \\ + \int \frac{d^3r}{4\pi} [E^2 + B^2 - 2\nabla\phi\{\frac{1}{c} \partial_t A + \nabla\phi\}] \qquad (2.2.12.)$$

where we have made use of the relations

$$P_\phi = 0$$

$$P_A = -E/4\pi c$$

$$P_r = mv + \frac{e_i}{c} A(r,t) \qquad (2.2.13.)$$

For future reference we observe that in general the canonical momentum P and the more physically relevant kinetic momentum

$$\pi_x \equiv m \frac{dx}{dt} = \frac{\partial H}{\partial P_x} = P_x - \frac{e_i}{c} A(r_x,t) \qquad (2.2.14.)$$

are different depending on the vector potential, and the kinetic momentum obeys modified commutation relations

$$[\pi_x,x] = \hbar/i; \quad [\pi_x, y] = \frac{-\hbar e}{ic} \{\partial_x A_y - \partial_y A_x\} \qquad (2.2.15.)$$

We will soon see it is important to specify which momentum is implicitly assumed in transport theory.

The general hamiltonian is reduced to our specific case by taking the potentials to be defined in terms of an arbitrary scalar function $\chi(r,t)$ by:-

$$A = \nabla\chi(r,t) \qquad (2.2.16.)$$

$$\text{and} \quad \phi = -\frac{1}{c} \partial_t \chi(r,t) - E_o(t)\cdot r \qquad (2.2.17.)$$

since upon substituting (2.2.16.) and (2.2.17.) into (2.2.10) yields respectively

$$B = 0$$

$$E(r,t) = E_o(t)$$

In terms of these potentials the Hamiltonian (2.2.12.) is just

$$H = \frac{1}{2m}\sum_i [P_i - \frac{e_i}{c}\nabla\chi(r_i,t)]^2 - \sum_i e_i[E_o\cdot r_i + \frac{1}{c}\partial_t\chi(r_i,t)]$$
$$- \int \frac{d^3r}{4\pi}[E^2 + \frac{2E}{c}\nabla\partial_t\chi(rt)] \qquad (2.2.18.)$$

Note that as long as the potentials are determined through (2.2.16.) and (2.2.17.) the Hamiltonian (2.2.18.) describes free electrons in a uniform electric field whatever choice of the arbitrary function $\chi(r,t)$ we make. This arbitrariness has no effect whatsoever on the physics and its' choice is known as a gauge condition which supplements the definitions (2.2.10.) to allow the electromagnetic potentials to be uniquely defined. This gauge choice is not restricted to the specialised case of uniform electric fields but is a general consequence of the invariance of (2.2.10.) under the transformation

$$\left.\begin{aligned} A &\to A - \nabla\chi \\ \phi &\to \phi + \frac{1}{c}\partial_t\chi \end{aligned}\right\} \qquad (2.2.19.)$$

Although any choice of $\chi(r,t)$ is physically allowed it is often convenient for any given problem to fix $\chi(r,t)$ in a certain form to reduce the mathematical complexity of (2.2.18.). With regards to our specific case, there are two gauge conditions in common usage which are:-

(a) $$\chi(r,t) = \text{constant} \qquad (2.2.20)$$

in which case from (2.2.16.) and (2.2.17.)

$$\left.\begin{aligned} A &= 0 \\ \text{and}\quad \phi &= -E\cdot r \end{aligned}\right\} \qquad (2.2.21.)$$

or (b) $$\chi(r,t) = -cr\cdot\int_0^t d\tau E(\tau)$$

$$\left.\begin{aligned} \text{so that}\quad A &= -c\int d\tau E(\tau) \\ \text{and}\quad \phi &= 0 \end{aligned}\right\} \qquad (2.2.23.)$$

For obvious reasons we will refer to the first of these choices (2.2.20.) as the ϕ-gauge (this is the one often assumed in interaction

problems where it is also known as the Coulomb gauge; it is also the gauge adopted in this thesis). The second choice (2.2.22.) we refer to as the A-gauge which is the one more often adopted in current theories utilising time dependent electric fields[48][49][73].

In either choice, the third term in the Hamiltonian (2.2.18.) is just a constant ($= \pm \int d^3r E^2/4\pi$) and thus is neglected being absorbed into the definition of the zero point of energy. Therefore the bottom line of this analysis is that the Hamiltonian describing our system may be written in the form

$$H = \frac{1}{2m} \sum_i [P_i - \frac{e_i}{c} A(r_i,t)]^2 + \sum_i e_i \phi(r_i,t)$$

where the canonical and kinetic momenta are different and the electromagnetic potentials are given explicitly by either

(a) $\qquad A = 0 \quad$ and $\quad \phi = - E(t) \cdot r$

or (b) $\qquad \phi = 0 \quad$ and $\quad A = - c \int_0^t d\tau E(\tau)$

One specific confusion that has arisen from the use of different gauges is that it has been insinuated[49] that the ϕ-gauge cannot conveniently handle time-dependent electric fields and that the A-gauge is altogether the best one to adopt in discussions of transport in strong electric fields[73]. This confusion is now resolved by studying the problem in both gauges.

If we consider first of all the A-gauge in which the Hamiltonian is just $\hat{H}_A = \frac{1}{2m} (\hat{\pi})^2$ where $\hat{\pi} = \hat{P} - e/c\, A(\hat{r},t) = \hat{P} + e/c \int_0^t d\tau E(\tau)$ it is clearly advantageous to solve the Schrödinger equation in the kinetic momentum representation where the wavefunctions $\psi_A(\pi,t) \equiv \langle \pi|\psi\rangle$ are obtained from

$$\langle \pi | i\hbar \partial_t | \psi \rangle = \langle \pi | \hat{H}_A | \psi \rangle = \varepsilon(\pi) \psi_A(\pi,t)$$

as $$\psi_A(\pi,t) = \psi_A(\pi,0)\exp\frac{-i}{\hbar}\int_0^t d\tau\varepsilon[\pi(\tau)] \qquad (2.2.24.)$$

where $\varepsilon(k) = k^2/2m$ and

$$\pi(t) = P + \frac{e}{c}\int_0^t d\tau E(\tau) \qquad (2.2.25.)$$

However in the ϕ-gauge where the Hamiltonian is just

$$\hat{H}_\psi = \frac{1}{2m}(\hat{P})^2 - eE\cdot\hat{r}$$

we would prefer to solve in the canonical momentum representation in which case Schrödingers equation may be expressed in the form

$$[\partial_t + eE\cdot\partial_p]\psi_\phi(P,t) = \frac{-i}{\hbar}\varepsilon(P)\psi_\phi(P,t) \qquad (2.2.26.)$$

This equation is solved by introducing the dimensional parameter τ through rewriting (2.2.25.) as

$$\frac{d\psi_\phi}{d\tau} = \frac{-i}{\hbar}\varepsilon[P(\tau)]\psi_\phi$$

which has the solution

$$\psi_\phi(P,t) = \psi_\phi(P,0)\exp\frac{-i}{\hbar}\int_0^t d\tau\varepsilon[P(\tau)] \qquad (2.2.27.)$$

where we have made use of the relations

$$\frac{dt}{d\tau} = 1 \quad \text{and} \quad \frac{dP}{d\tau} = eE \quad \text{or} \quad P(\tau) = P + \int_0^\tau dt' eE(t').$$

Since at $t = 0$ the electric field is zero we must have

$$\psi_\phi(0) = \psi_A(0)$$

which are in fact plane wave states being solutions of the free electron Hamiltonian. Therefore we see that the momentum wavefunctions calculated in the two different gauge representations are the same

i.e. $$\psi_\phi(P,t) = \psi(0)\exp\frac{-i}{\hbar}\int_0^t d\tau\varepsilon[P(\tau)]$$

$$\equiv \psi_A(\pi,t)$$

where $P(\tau)$ is given by (2.2.25.) although the 'momentum' utilised in both cases refers to different animals being the kinetic and canonical momenta respectively.

The difference in wavefunctions due to the two gauge choices may be seen in the position representation of the wave function obtained by the momentum expansions:-

$$\psi_\phi(r,t) = \sum_P \langle r|P\rangle\psi_\phi(P[t]) \qquad (2.2.28.)$$

and $$\Psi_A(r,t) = \sum_\pi \langle r|\pi\rangle\Psi_A(\pi[t]) \qquad (2.2.29.)$$

where $$\langle r|P\rangle = \text{constant x } \exp\frac{i}{\hbar}P\cdot r \qquad (2.2.30.)$$

and $$\langle r|\pi\rangle = \text{constant x } \exp\frac{i}{\hbar}\pi\cdot r \qquad (2.2.31.)$$

$$= \text{constant x } \exp\frac{i}{\hbar}r\cdot[P + \int_0^t d\tau eE(\tau)]$$

Therefore since the momentum wavefunctions are the same in the two gauges (essentially because the energy eigenvalues, being observables, must be independent of the gauge choice) we can see on substituting (2.2.31.) into (2.2.29.) that the wavefunctions in the two gauges in the position representation are related by

$$\psi_A(r,t) = \exp[\frac{i}{\hbar}r\cdot\int_0^t d\tau eE(\tau)]\psi_\phi(r,t) \qquad (2.2.32.)$$

The transformation (2.2.32.) has been used by Pottier and Calecki[73] and Jauho[49] in the analysis of field dependent transport to convert results in the presumed simpler A-gauge into the ϕ-gauge representation. The reason for the assumed simplicity in the A-gauge is that it yields

explicitly field dependent energy eigenvalues (through the kinetic momentum) and thus illustrates that scattering, induced by some small perturbation, takes place between accelerating momentum eigenstates due to the action of the field within a collision process. However the same results may be easily obtained using the ϕ-gauge as we have just illustrated thus repudiating any claim that the ϕ-gauge is in any sense unsuitable. In fact an argument exists in favour of the ϕ-gauge over the A-gauge even in this simple case because in the A-gauge the Hamiltonian is independent of the position variable. This consequence led Poitier and Calecki[73] to claim that the application of a uniform electric field does not destroy the translational invariance of the system and so the appearance of the $E\cdot r$ term in the ϕ-gauge Hamiltonian must be an indication of the unsuitability of this gauge. However, it is clear that it is precisely the reverse that is true in that even a uniform field will make a system inhomogeneous because work must be performed on an electron in moving it from one place to another. The confusion arises because in quantum mechanics the symmetry of the system is not determined solely by the Hamiltonian operator, but the pair (H,ψ) and as may be seen in (2.2.32.) even if a suitable gauge choice should make H independent of r, the spatial variation will have been shifted into the gauge dependent wavefunction. This confusion would not have arisen if the ϕ-gauge was employed. (Of course, in more complicated situations where the electron-electron interaction is included, the ϕ-gauge is certainly preferable to the A-gauge because usually the inter-particle bare Coulomb interaction which varies as $1/|r|$ is calculated under the inherent assumption of the ϕ-gauge, a point which will be emphasised in §4.1.)

Although the transformation (2.2.32.) was obtained by specific calculations, we would expect such a relationship by demanding gauge

invariance of the Schrodinger equation under an arbitrary electromagnetic field, since invariance of the equation

$$i\hbar\partial_t|\psi> = [\frac{1}{2m}(\frac{\hbar}{i}\nabla - \frac{e}{i}A)^2 + e\phi]|\psi>$$

under transformations (2.2.18.) demand that the wavefunctions be simultaneously transformed as

$$\psi \rightarrow \psi' = e^{i\Omega(r,t)}\psi$$

where $\Omega(r,t) = -e\chi(r,t)/\hbar c$, $\chi(r,t)$ being the chosen gauge function. Therefore in the transformation from the ϕ-gauge to the A-gauge for a uniform electric field (for which $\chi(r,t) = -cr\cdot\int_0^t d\tau E(\tau)$) the new wave function is obtained from the old by the unitary transformation

$$\psi' = \psi\exp[\frac{ie}{\hbar}r\cdot\int_0^t d\tau E(\tau)]$$

which is precisely the content of (2.2.31.) obtained by an explicit calculation in both gauges.

Thus far we have outlined and corrected some of the misunderstandings common in the wavefunction approach. We will now return to our original aim of calculating scattering transition rates by using the wavefunctions (2.2.27.) to calculate the matrix elements in (2.2.6.).

To this end we consider the perturbation as being due to an electron-phonon interaction where the perturbation may be expressed in the form $V(r,t) = \sum_q M(q)e^{iq\cdot r \pm i\omega_q t}$ where $M(q)$ measures the strength of the interaction for a momentum transfer of $q = p' - p$ to an emitted (absorbed) phonon of energy $-(+)\hbar\omega_q$. Employing this form of the scattering potential along with the complete set of wavefunctions (2.2.27.) for free electrons in a uniform electric field gives an expression for the scattering rate (2.2.6.) which may be written in the form

$$R_{p\to p'}(t) = 2\frac{|\tilde{M}|^2}{\hbar^2}\,\mathrm{Re}\int_0^t d\tau\{\exp\frac{i}{\hbar}\int_t^\tau dt'[\varepsilon(P' + \int_0^{t'} dt''eE(t'')) - \varepsilon(P + \int_0^{t'} dt''eE(t''))] \pm i\omega_q(\tau - t)\} \qquad (2.2.33.)$$

where $\tilde{M}(q)$ are the scattering matrix elements evaluated between plane wave states. In the simple case of a constant electric field, and a quadratic energy dispersion relation, (2.2.33.) reduces to the succint form

$$R_{p\to p'}(t) = \frac{2|\tilde{M}(q)|^2}{\hbar^2}\,\mathrm{Re}\int_0^t d\tau e^{\frac{i}{\hbar}[\Delta_0(t-\tau)+\Delta_1(t^2-\tau^2)]} \qquad (2.2.34.)$$

where $\Delta_0 = \varepsilon(P') - \varepsilon(P) \pm \hbar\omega_q$

and $\Delta_1 = \frac{eE\cdot(P' - P)}{2m}$

It is straightforward to show that the zero field asymptotic ($t \to \infty$) limit of (2.2.34.) is just

$$\frac{2\pi}{\hbar}|\tilde{M}|^2\delta[\varepsilon(P') - \varepsilon(P) \pm \hbar\omega_q]$$

which is recognisable as the conventional Golden rule structure used to obtain transition rates. Consequently for non zero electric fields it is reasonable to interpret (2.2.34.) as a generalised Golden rule where, as a consequence of the strong fields the usual sharp δ-function form of energy conservation has been broadened and displaced, and since only a finite time is allowed for the scattering event the transition rate involves only a finite time integral. We remark that the infinite time limit of (2.2.34.) is precisely the result obtained by Barker[9][10] and Thornber[91] using alternative techniques for a generalised Golden rule. We also emphasise that it is not equivalent to the recent results of Herbert and Till[40][41] who used the same approach as presented here but utilised the alternative definition of a transition rate (2.2.7.).

The consequences of (2.2.33.) and (2.2.34.) are the main achievements of the wavefunction approach since they demonstrate that in high field transport the electric field should contribute explicitly to the collision integrals at least through the transition rates. The conventional structure is only obtained in the zero-field asymptotic limit which corresponds to calculating the transition rate between stationary eigenstates.

In order to obtain a complete transport theory we must now use this transition rate to construct a kinetic equation for the electron distribution function. Denoting the transition rate as[82]

$$R_{p\to p'} = \frac{2|M|^2}{\hbar^2}\int_0^t d\tau \Gamma_{pp'}$$

a construction of the total scattering integral has been made by convolving $R_{p\to p'}$ with the kinetic bracket of the scattering processes in question. The resulting transport equation is

$$\partial_t f(\pi) = \frac{2}{\hbar^2}\sum_{p',q}|\tilde{M}(q)|^2\int_0^t d\tau\{L^{(+)}_{pp'}(t-\tau)\Gamma_{pp'}(\tau) + L^{(-)}_{pp'}(t-\tau)\Gamma_{p'p}(\tau)\} \qquad (2.2.35.)$$

where the kinetic bracket $L^{(\pm)}_{pp'}$ is just

$$L^{(\pm)}_{pp'} = [1-f(\pi)]f(\pi')[N_q + \tfrac{1}{2} \pm \tfrac{1}{2}] - f(\pi)[1-f(\pi')][N_q + \tfrac{1}{2} \mp \tfrac{1}{2}] \qquad (2.2.36.)$$

$\pi = p + eE\tau$, and N_q is the phonon distribution function.

To obtain this transport equation it has had to be assumed that $f(\pi) = f(\pi,\tau)$ and $N(q) = N(q,\tau)$ in order that the transition rate and the kinetic bracket may be combined in a convoluted integral structure. It is not obvious that this ad hoc procedure is a correct description of the dynamics and moreover it is not clear that the kinetic bracket must be

of the form (2.2.36.). These queries are merely indicative that the wavefunction approach to transport phenomena is inadequate to deal correctly with many body quantum dynamical transport. It is unable to incorporate many body effects properly, a complete kinetic equation may only be obtained using phenomenological arguments and the calculation of transition elements, which may be deemed its' strong point, may only be performed assuming very simple systems far removed from submicron devices.

However we have seen that the method does serve to illustrate specific effects that may be expected to modify our conventional view of transport. In particular we refer to the generalised Golden rule form (2.2.33.) which is modified by the non-asymptotic time structure and its' explicit dependence on the electric field. The first phenomenon is a consequence of the scattering proceeding between non-stationary states and the second due to the action of the field within a collision process. Both effects should contribute to replace the sharp energy conservation factors by a broadened and displaced function. Whether such features will remain in a more rigorous approach to the transport problem is discussed in Chapter IV.

§2.3. The equation of motion technique

The third and final typical approach to quantum transport we consider is known as the kinetic equation, or equation of motion method. We have seen in the preceding section that although the wavefunction approach manages to incorporate the electric field in the collision integral, it is not sufficiently powerful to incorporate consistently many body effects due primarily to the electron-electron interactions in particular. We shall see that the equation of motion method attempts to incorporate such many body effects in a systematic manner although it suffers from the increased mathematical complexity of the resulting equations.

The general technique is borrowed from a method devised to deal with dilute plasmas which was pioneered (alphabetically and anti-chronologically) by Bogolyubov[16], Born[18], Green[18], Kirkwood[52] and Yvon[101] and may be described as follows.

One considers the equation of motion of the single particle distribution function (suitably defined) derived from an assumed model Hamiltonian. Since this Hamiltonian should in general involve particle-particle interactions, the single particle equation of motion will be explicitly dependent on the two particle distribution function (and mixed particle distribution functions if the interaction is between unlike objects such as electrons and phonons). Consequently to solve the single particle equation it is necessary to solve the two-particle equation which in turn will depend on the three particle distribution function. In this fashion the interactions generate an infinite set of coupled equations of motion which has become known as the "BBGKY hierarchy" after the aforementioned pioneers of the technique.

The method of solving this infinite set of equations is to introduce correlation functions at each level of the hierarchy and then assume it is a good approximation to neglect the correlations above some given order. In this way one obtains a finite set of equations which it is hoped may be consistently reduced to just one equation for the single particle distribution function under certain additional simplifying assumptions. Therefore, depending on the level of truncation of this hierarchy, the method is capable of incorporating many body effects to any desired order. Unfortunately the equations are generally so complicated to solve that the truncation procedure has to be made at a very low order and typically no more than the two-particle level[3][10][19][63][79][83][99].

It is best to illustrate these remarks with a specific example based on an electron assembly interacting via a two body potential $\phi(r_1-r_2)$ where we assume the Hamiltonian involving the electron annihilation (ψ_s) and

creation ($\psi_s^\dagger$) operators of spin s is given by

$$\hat{H} = \sum_s \int d^3r\psi^\dagger(r)\{\frac{-\hbar^2}{2m}\partial_r^2 +$$

$$+ \tfrac{1}{2}\sum_{s'}\int d^3r'\psi^\dagger_{s'}(r')\phi(r-r')\psi_{s'}(r')\}\psi_s(r) \qquad (2.3.1.)$$

The relevant n-particle distribution functions in this case are averages of the density matrix defined as

$$F_{s_1,s_2\,..\,s_n}(1'2'..n';1,2..n) =$$

$$<\psi^\dagger_{s_1}(r,t)..\psi^\dagger_{s_n}(r_n,t)\psi_{s_n}(r_n t)..\psi_{s_1}(r,t)> \qquad (2.3.2.)$$

where in the Heisenberg representation

$$<\hat{A}> = Tr[\hat{A}\rho]$$

and $\rho \equiv \rho(t = 0)$ is the equilibrium density matrix given by the grand canonical ensemble.

Using the Heisenberg equation for an arbitrary operator $\hat{A}$

$$i\hbar\partial_t\hat{A} = [\hat{A},\hat{H}]$$

the one-and two-electron equations of motion may be obtained as

$$[i\hbar\partial_t + T(11')]F_{s_1}(1';1) =$$

$$\sum_{s_2}\int d^3r_2[\phi(r_1-r_2) - \phi(r_1'-r_2)]F_{s_1s_2}(1'2;12) \qquad (2.3.3.)$$

and

$$[i\hbar\partial_t + T(11') + T(22') + \phi(r_1-r_2) - \phi(r_1'-r_2')]F_{s_1s_2}(1'2';12)$$

$$= \sum_{s_3}\int d^3r_3[\phi(r_1-r_3) - \phi(r_1'-r_3) + \phi(r_2-r_3) -$$

$$- \phi(r_2'-r_3)]F_{s_1s_2s_3}(1'2'3;123) \qquad (2.3.4.)$$

where T(11') is the kinetic operator $\hbar^2/2m[\partial^2 r_1 - \partial^2 r_{1'}]$.

Therefore in this specific example we see that the one particle equation of motion (2.3.3.) depends on the two-particle distribution the equation of motion (2.3.4.) of which is governed by the three particle distribution. Clearly (2.3.3.) and (2.3.4.) represent the lowest rungs of an infinite BBGKY hierarchy, and are generated by any two body interaction considered since we have not made explicit use of the fact that $\phi(r)$ represents the Coulomb interaction in this specific case. Thus for example if we considered interactions between electrons and non-polar phonons represented by annihilation and creation operators $b, b^\dagger$ we would have obtained a single electron equation of motion involving the mixed correlation functions $\langle b^\dagger \psi^\dagger \psi \rangle$ and $\langle b \psi^\dagger \psi \rangle$ which would introduce a further branch into the hierarchy[79].

The reduction of such an unmanageable hierarchy is to follow the lead of classical equilibrium statistical mechanics where it is found useful to expand the distribution functions in terms of irreducible correlation functions - a procedure known as the Meyer cluster expansion (see for example [66]). In particular the two-and three-particle correlation functions (g,h) are defined through

$$F_1 = F_1$$

$$F_2 = F_1 F_1 + g \qquad (2.3.5.)$$

$$F_3 = F_1 F_1 F_1 + \sum F_1 g + h \qquad (2.3.6.)$$

where the sum in (2.3.6.) runs over cyclic permutations of the co-ordinates. Consequently g is determined through the equation of motion of F_2 and h through the equation of F_3 and so on.

The resulting infinite set of equations for the correlation functions is truncated to a finite set by neglecting all correlations above some given order. Typically the choice is $h = 0$ because even though this does

manage to include two particle correlation effects (such as screening) and neglect three particle correlations the resulting pair of equations is still too difficult to solve. To illustrate this in our specific case we introduce a slightly different definition of the correlation function (g) i.e.

$$F_{s_1s_2}(1'2';12) = \gamma_2[F_{s_1}(1';1)F_{s_2}(2';2) + g_{s_1s_2}(1'2';12)] \quad (2.3.7.)$$

where the symmetrisation operator[77]

$$\gamma_2 = [1 - \delta_{s_1s_2}\hat{P}_{12}]$$

ensures exchange effects are included ($\hat{P}_{12}$ permutes the variables $r_1 \leftrightarrow r_2$). Assuming $h = 0$ and using (2.3.7.) in (2.3.4.) gives an equation for the correlation function of a homogeneous electron assembly of

$$\begin{aligned}
&[i\hbar\partial_t + T(11') + T(22') + \phi(r_1-r_2) - \phi(r_1'-r_2)]g(1'2';12) \\
&= [\phi(r_1-r_2) - \phi(r_1'-r_2)]F_{s_1}(r_1'-r_1)F_{s_2}(r_2'-r_2) \\
&+ \sum_{s_3}\int d^3r_3\{[\phi(r_1-r_3) - \phi(r_1'-r_3)]F_{s_1}(r_1'-r_1)g_{s_2s_3}(2'3;23) \\
&+ [\phi(r_2-r_3) - \phi(r_2'-r_3)]F_{s_2}(r_2'-r_2)g_{s_1s_3}(1'3;13) \\
&- \sum_{s_3}\int d^3r_3d^3r_3'\delta(r_3-r_3')\{[\phi(r_1-r_3) - \phi(r_1'-r_3)]\delta_{s_2s_3}P_{23} \\
&+ [\phi(r_2-r_3) - \phi(r_2'-r_3)]\delta_{s_1s_3}P_{13}\} \\
&\times F_{s_1}(r_1'-r_1)F_{s_2}(r_2'-r_2)F_{s_3}(0) \qquad (2.3.8.)
\end{aligned}$$

This equation along with (2.3.3.) (and using (2.3.7.)) constitutes a pair of coupled closed equations of motion. The procedure now is to solve (2.3.8.) for the two particle correlation function and substitute into (2.3.3.) to give one single electron equation of motion capable of describing two-body correlations. However the obvious complexity of (2.3.8.) makes this impossible unless we assume the single electron

distribution function varies slowly with respect to the correlation function and we only need to consider the zeroth order terms of (2.3.8.)[10], equivalent to assuming that the electron system reacts instantaneously to the movement of a single electron.

This is a very complicated procedure[79][99] and so is not pursued further other than to note that it is only a workable method under extremely restrictive conditions. The situation is proportionally more difficult when the system cannot be considered as homogeneous (for example when the application of a uniform electric field destroys the translational symmetry) or when additional scattering mechanisms are taken into account thus increasing the number of coupled equations to solve even at the lowest order of truncation. However, even if the resulting set of equations was simple to solve there is still a fundamental difficulty associated with the ansatz of neglecting n-th and higher order correlations for some given n.

If we return to (2.3.5.) we may appreciate the physical basis of such an ansatz since we know that at large distances two particles may be considered as uncorrelated in which case their joint distribution function is just the product of independent distributions. Therefore expressing F_2 as F_1F_1 + g gives an interpretation of the correlation function as being roughly proportional to the ratio between potential and kinetic energies per particle. Hence the more particles involved in the correlation the less significant is that correlation function when compared to lower order correlations since there is a reduced probability of finding all the particles close together. Given this argument it seems physically obvious that it would be a good approximation to neglect n-th order and higher correlation functions if we are only interested in (n - 1)-particle effects.

However, from a mathematical viewpoint this procedure is equivalent to making the cumulant generating function[53] of the distribution an

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However, from a mathematical viewpoint this procedure is equivalent to making the cumulant generating function[53] of the distribution an

exponential of a finite polynomial. According to a theorem due to Marcinkiewicz[62], in order to be consistent with classical probability theory this polynomial may be no more than quadratic and thus if we assume the n-th order correlation function is zero for some $n > 2$, we must necessarily have that *all* correlations above second order are zero.

This poses a severe restriction on truncation schemes in physics since it states that as long as we are content with a theory described by the first two moments then we can obtain consistent results. However if we wish to expand our horizons to include higher moments then we are forced to include all such moments in some fashion. This is a surprising and unexpected result which is so relevant to transport theory that the next chapter is devoted to a discussion of this theorem and its' consequences with regards to quantum distribution functions.

In spite of this technical objection we remark that the equation of motion method is the most systematic (although complicated) procedure used to date (with the exception of a functional derivative technique developed in Chapter IV) to tackle non-equilibrium quantum transport which makes a serious attempt to incorporate many body effects consistently.

Thus to summarise this chapter we have examined three typical approaches to the modelling of high field quantum transport. Each has their respective merits and faults: the phenomenology and lack of precision in the Boltzmann equation approach is countered by the valuable physical insight brought to the subject by its' various model solutions; the wave function approach suffers from ambiguities in the definitions of how a transport equation should be constructed although its handling of a uniform electric field exhibits new features that ought to be introduced in a transport theory and the equation of motion method, although attempting to incorporate many body effects properly, is too cumbersome a technique to exploit the dynamic effects of strong inhomogeneities.

In short, no single approach considered is capable of accurately

describing the high field quantum transport in sub-micron devices although each theory offers an aspect we would find attractive in a more complete theory.

CHAPTER 3

QUANTUM MECHANICAL DISTRIBUTION FUNCTIONS: THE WIGNER FUNCTION AND THE MARCINKIEWICZ THEOREM

§3.1. Introduction

Generally speaking, contemporary quantum transport physics is performed assuming the state space interpretation of quantum mechanics. This is because historically, in order to incorporate the existence of discrete energy levels in systems described by Hamiltonians which were continuous functions of position and momentum, it was found necessary to introduce an algebra of non-commuting Hermitian operators which acted on vectors in some state-space[81].

Within this context the state of a particular system is characterised by a vector (denoted by $|\psi>$) in this space; observable quantities by Hermitian operators $\hat{S}$, and the allowed values (S) that any measurement of this observable may yield are obtained from an eigenvalue equation

$$\hat{S}|\psi> = S|\psi> \qquad (3.1.1.)$$

which, upon using the completeness relation

$$\int d\tau \psi^*(\tau)\psi(\tau) \equiv <\psi|\psi> = 1 \qquad (3.1.2.)$$

yields

$$S = <\psi|\hat{S}|\psi> \qquad (3.1.3.)$$

where $<\psi|$ are vectors in the conjugate space to the one defined by $|\psi>$.

This description corresponds to the "pure state" situation where we know that our system is in a particular state $|\psi>$. Of course in general we can only assign a statistical probability P_n of the system being in any given state $|\psi_n>$ and so if the corresponding eigenvalue is S_n we have

a statistical interpretation of the average value of an observable denoted by

$$\langle\hat{S}\rangle = \sum_n P_n S_n = \sum_{n,m} \langle\psi_m|P_n|\psi_n\rangle\langle\psi_n|\hat{S}|\psi_m \qquad (3.1.4.)$$

$$\equiv Tr[\hat{\rho}\hat{S}] \qquad (3.1.5.)$$

where (3.1.5.) defines the statistical density matrix

$$\hat{\rho} = \sum_n P_n|\psi_n\rangle\langle\psi_n| \qquad (3.1.6.)$$

that totally characterises the system. This density matrix is the central object in quantum theory viewed from the state-space interpretation: it is the most general representation of a quantum mechanical system and once given may be used to calculate the expectation value of observables through (3.1.4.) by summing the leading diagonal of the matrix product of the density matrix with the matrix of the operator corresponding to the observable.

However this state-space interpretation is alienated from the phase space description that has been used so successfully in classical mechanics. In this picture the state of a system is represented by a point in a 6N-dimensional phase space of the co-ordinates and momenta of the N-particle system. In terms of this phase space a distribution function f(r,p,t) may be introduced as the density of phase points in terms of which the expected value of an observable (now represented by a function A(r,p) of the phase space co-ordinates) is calculated in the conventional sense of a statistical ensemble, i.e.

$$\langle A\rangle = \int dpdqA(p,q)f(p,q,t) \qquad (3.1.7.)$$

Therefore if we know the distribution function we can calculate any relevant system observable and so in terms of dynamics the distribution could be obtained in principle from a transport equation such as the one

introduced by Boltzmann.

The difference in the two interpretations of the framework of quantum and classical mechanics are summarised in Table 3.1.1.

APPROACHES	CLASSICAL	QUANTUM
Base space components	Phase-space points (p,q)	State-space vectors $\|\psi\rangle$
Space densities	Distribution function $f(pqt)$	Statistical density matrix $\hat{\rho}$
Liouvilles equation of motion	$\partial_t f = \sum_{i=1}^{N} [\partial_{q_i} f \partial_{p_i} H - \partial_{p_i} f \partial_{q_i} H]$	$\partial_t \hat{\rho} = \frac{1}{i\hbar} (\hat{H}\hat{\rho} - \hat{\rho}\hat{H})$
Expected value of observable quantities	$\int dpdqA(pq)f(pqt)$	$Tr[\hat{A}\hat{\rho}]$

TABLE 3.1.1.

Obviously the algebras governing quantum and classical mechanics are different, however comparisons between the two are complicated due to the algebras operating on different types of basis space. Therefore to explicitly exhibit differences in the dynamics of quantum and classical mechanics it would be preferable to look at the action of the two algebras on the *same* basis space[17]. If we choose to look at the problem from a unified point of view based on the phase space interpretation then the hope must be that some of the many techniques both analytic and numerical, developed for classical transport theory (and particularly with regard to the Boltzmann equation) may be transposed successfully to analyse quantum transport problems.

Before we consider quantum transport theory in phase space (Chapter 4) we need to discuss a few problems associated with general quantum mechanical phase space distributions since we already know they cannot

have the same interpretation as classical distributions due to the function referring to specific momentum and position values at the same time - something against the spirit of the uncertainty relations.

In order to introduce quantum distributions it is useful to first consider the relevance to physical transport theories of a mathematical theorem due to Marcinkiewicz[62]. This theorem is illustrated in the next section where the implications are discussed as a need to relax some of the inherent restrictions we impose on classical distribution functions.

§3.2. The Marcinkiewicz Theorem

We have already noted in §2.3. that a large class of physical transport theories involve the reduction of an infinite set of coupled equations (the BBGKY hierarchy) to a finite number by the complete neglect of high order correlations between many particles. However as was first pointed out by Robinson[78] and later discussed by Rajagopal[75], Sudarshan[75] and Titulaer[93], this procedure in general violates a mathematical theorem proposed by Marcinkiewicz[62] in 1938 which may be stated in the following terms.

The theorem refers to the behaviour of a quantity known as the characteristic or moment generating function C(t) which is defined as the expectation value of exp[itx] where x is a generalised random variable (which in quantum mechanics may be interpreted as a q-number[53])

i.e.
$$C(t) = \langle \exp[itx] \rangle$$
$$\equiv \sum_{n=0}^{\infty} \frac{(it)^n}{n!} \mu_n \qquad (3.2.1.)$$

where $\mu_n = \langle x^n \rangle$ is the n-th moment of the distribution. Expression (3.2.1.) may be used to define the n-th cumulant κ_n by expressing it in terms of the cumulant generating function $\kappa(t)$ as

$$C(t) = \exp K(t)$$

$$\equiv \sum_{n=1}^{\infty} \frac{(it)^n}{n!} \kappa_n \qquad (3.2.2.)$$

The cumulants are not simple averages but may be expressed in terms of lower order moments by equating the coefficients in the respective expansions of (3.2.1.) and (3.2.2.), for example

$$\kappa_2(x_1,x_2) = \langle x_1x_2\rangle - \langle x_1\rangle\langle x_2\rangle \qquad (3.2.3.)$$

$$\kappa_3(x_1,x_2,x_3) = \langle x_1x_2x_3\rangle$$

$$- \{\langle x_1\rangle\langle x_2x_3\rangle + \langle x_2\rangle\langle x_3x_1\rangle + \langle x_3\rangle\langle x_1x_2\rangle\}$$

$$+ 3\langle x_1\rangle\langle x_2\rangle\langle x_3\rangle \qquad (3.2.4.)$$

Therefore we see that the cumulants are what is physically known as correlation functions and the truncation schemes mentioned in §2.3. usually relied on the assumption that $\kappa_3 = 0$ in (3.2.4.) where the random variable x referred to the local density of electrons.

If F(x) is the corresponding probability density to the random variable x, then the definition of the characteristic function (3.2.1.) may be written in terms of the probability density as

$$C(t) = \langle \exp[itx]\rangle$$

$$\equiv \int_{-\infty}^{\infty} \exp[itx]dF(x) \qquad (3.2.5.)$$

which upon inverting furnishes a definition of the distribution function f(x) in terms of the characteristic function:

$$f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \exp[-itx]C(t)dt \qquad (3.2.6.)$$

Therefore in this scheme the characteristic function is considered as a fundamental quantity with respect to which the distribution function

is a secondary defined quantity.

One particularly important example of a characteristic function is

$$C_N(t) \equiv \exp[iat - \tfrac{1}{2}\sigma^2 t^2] \qquad (3.2.7.)$$

and in which case its' corresponding probability density is just the normal distribution[59]

$$F_N(x) = \frac{1}{\sqrt{2\pi\sigma}} \exp[-(x - a)^2/2\sigma^2] \qquad (3.2.8.)$$

We now come to a statement of the Marcinkiewicz theorem which, in terms of the characteristic function, says that if the cumulant generating function is a polynomial then to be consistent with conventional probability theory this polynomial must necessarily be no more than quadratic. In other words if there are only a finite number of non-zero correlation functions then *all* correlations above second order must be taken to be zero.

The implications of this theorem with regards to truncation schemes in many body approximations are clear: as long as one is content with a transport theory defined by the first two moments of the random variable considered, then consistent results may be obtained. However this consistency will be lost if attempts are made to extend the theory by including a finite number of non-zero higher order moments. Therefore it would appear that the most general situation that may be accurately described by using the truncation technique is a generalised free field model given by the displaced Maxwellian akin to (3.2.8.). Although this represents a very strong argument against the use of terminating the BBGKY hierarchy in such a fashion, the limitations imposed by this theorem have largely been ignored in the literature.

The theorem also has consequences with regards to the construction of quantum mechanical phase space distribution functions but in order to see why it is necessary to rederive the Marcinkiewicz theorem using concepts more familiar to physicists than the pure mathematician.

First of all, if we consider what useful properties characterise a distribution function then by analogy with classical mechanics we would perhaps impose the three minimal requirements that the distribution function be

$$\left.\begin{array}{ll} \text{(a)} & \text{Real} \\ \text{(b)} & \text{Bounded (in the sense that } \int dF(x) \text{ is finite)} \\ \text{and} & \text{(c)} \quad \text{Non-negative} \end{array}\right\} \qquad (3.2.9.)$$

Therefore we would also suppose that these three conditions represent restrictions on the behaviour of the characteristic function defining the distribution function and indeed these restrictions may be derived as follows.

We see from (3.2.6.) that if the distribution function is real then the characteristic function must be Hermitian i.e.

$$\text{(a1)} \qquad C^*(t) = C(-t) \qquad (3.2.10.)$$

Secondly if the distribution function is bounded (which we would require in the quantum mechanical case so that the projections in momentum and position may be regarded as true probability distributions) it follows from (3.2.5.) that C(t) is also bounded and moreover

$$\text{(b1)} \qquad |C(t)| \leq \int |dF(x)| = 1 \qquad (3.2.11.)$$

if f is non-negative

The third requirement on the distribution function, that of non-negativity implies that the equality in (3.2.11.) holds *only* for t = 0 i.e.

$$\text{(c1)} \qquad |C(t)| = 1 \quad \textit{only} \text{ at } t = 0. \qquad (3.2.12.)$$

This latter restraint is not obvious but may be illustrated as follows. From (3.2.5.) we have

$$|C(t)|^2 = [ReC(t)]^2 + [ImC(t)]^2$$

$$\leq \int \cos^2 txdx \int f^2(x)dx + \int \sin^2 txdx \int f^2(x)dx$$

by the Schwartz Inequality[90] where the equality only holds if the function $g(x)$ (= costx or sintx) is directly proportional to $f(x)$ or is altogether independent of x, in which case we must have $t = 0$ at which value

$$|ReC(t)| = \int |f(x)|dx \qquad (3.2.13.)$$

and

$$|ImC(t)| = 0 \qquad (3.2.14.)$$

Since we are assuming that the distribution function is non-negative we must have

$$\left|\int dF(x)\right| = \int |dF(x)| = 1 \qquad (3.2.15.)$$

so that through (3.2.13.) we have the restriction (c1), i.e. that $|C(t)| = 1$ only at $t = 0$.

Note that (c1) need not be true if the distribution function is allowed to assume negative values since then

$$\int |dF(x)| > \left|\int dF(x)\right| = 1 \qquad (3.2.16.)$$

which would permit $|C(t)|$ to be greater than unity for a range of t values and consequently it would be possible for $|C(t)|$ to equal unity at values of t other than zero.

Therefore to reiterate we recognise that the three physically reasonable requirements (3.2.9.) impose three constraints (a1)-(c1) on the behaviour of the characteristic function. We will now see that these three constraints are sufficient to generate the Marcinkiewicz theorem.

We have seen that the characteristic function may be expanded in terms of correlation functions through

$$C(t) = \exp \sum_{n=1}^{\infty} \frac{(it)^n}{n!} \kappa_n$$

Consequently if we assume only a finite number of correlations are involved so that

$$C(t) = \exp P(t)$$

where $P(t)$ is a polynomial of the form

$$P(t) = \sum_{n=1}^{N} \frac{(it)^n}{n!} \kappa_n$$

$$= itQ(t^2) - t^2R(t^2) \qquad (3.2.17.)$$

and Q, R are polynomials in t^2, then restrictions (a1)-(c1) may be used to determine the precise form of Q, R as follows.

Since we know $C(t)$ is Hermitian (a1), then Q and R must be polynomials with real coefficients (in other words the correlations themselves are real). Consequently the real and imaginary parts of the characteristic function may be expressed as

$$\mathrm{Re}C(t) = \exp[-t^2R(t^2)]\cos[tQ(t^2)] \qquad (3.2.18.)$$

$$\mathrm{Im}C(t) = \exp[-t^2R(t^2)]\sin[tQ(t^2)] \qquad (3.2.19.)$$

Moreover, since the magnitude of $C(t)$ is governed by $\exp[-t^2R(t^2)]$ and we know from (b1) that $|C(t)| \leq 1$, we must ensure that $R(t^2)$ cannot assume a negative value for any choice of t and consequently we must infer that $R(t^2)$ is a real polynomial with *positive* coefficients.

We now impose condition (c1) on (3.2.18.) and (3.2.19.) in two stages. First we recall from (c1) that $t = 0$ is the only value of t for which $|\mathrm{Re}C(t)| = 1$ and so from (3.2.18.) if

$$|\mathrm{Re}C(t)| \equiv \exp[-t^2R(t^2)]$$

equals unity only at $t = 0$, then we need to ensure that $R(t^2)$ has no roots.

The only conclusive way of ensuring this is to assume that $R(t^2) = r_0 =$ constant for all t.

Similarly if t = 0 is the only solution that satisfies ImC(t) = 0 then from (3.2.19) to be sure $Q(t^2)$ has no roots it is necessary to take $Q(t^2) = q_0 =$ constant.

Therefore combining the restrictions on (3.2.17.) due to the conditions (a1)-(c1) leads to a characteristic function of the form

$$C(t) = \exp[iq_0 t - r_0 t^2] \qquad (3.2.20.)$$

where q_0, r_0 are real constants and r_0 is positive, i.e. the characteristic function must be the exponential of a quadratic polynomial which is precisely a restatement of the Marcinkiewicz theorem. Indeed (3.2.20.) is identical to the characteristic function of the normal probability density (3.2.7.) even down to the prediction of the correct sign of r_0 (which being positive may be written in the form of $\frac{1}{2}\sigma^2$ say).

We note that although the original proof of the Marcinkiewicz theorem relied on involved mathematics[62] the construction just presented depends only on the three physically reasonable restraints (3.2.9.) which have been borrowed from our knowledge of classical distribution functions. Consequently it is not difficult to see that the Marcinkiewicz theorem presents a severe restriction on the construction of quantum distribution functions in general which may be expanded in these terms: if we require a real, bounded, non-negative distribution function constructed out of a finite number of correlation functions, then the only probability density we are allowed is the normal distribution, being constructed out of the first two moments only.

This is evidently far too restrictive for practical purposes and yet is a direct consequence of requiring that the distribution function satisfy the three apparently reasonable constraints (3.2.9.).

Of course in quantum dynamical systems, even if we could initialise a distribution function to be in this restrictive form, its' subsequent evolution (under an electric field for instance) would progressively

involve higher moments than second order due to the interactions within a system from both collisions with other particles and the interactions with the inbuilt system potentials such as boundaries and static charge inhomogeneities introduced by doping for example. Moreover we could only ever be aware of a finite number of these moments because if we had the information of all moments we would know everything about our system which is against the fundamental issues of quantum mechanics, and herein lies the contradiction with the Marcinkiewicz theorem.

We can see that in order to reconcile the construction of a quantum distribution function with this theorem, we are forced to relax at least one of the prejudices in (3.2.9.) inherent in classical distribution theory. The choice we will use in this thesis is to take a real, bounded distribution function which by the foregoing discussion must in general be allowed to assume negative values. This particular choice is the Wigner distribution function[97] to be constructed in the next section.

It is important to recognise that the construction of a quantum distribution function is not unique; it would be perfectly feasible to construct a quantum distribution function which was always positive for example[44] but if we required it to be bounded, then it would also in general have to be a complex valued quantity. The construction may only be made unique by the additional imposition of a set of extra restraints. This lack of uniqueness is not surprising since the only significance of a distribution function is its' use in calculating the correct average values of observable quantities - as long as the calculations lead to the same value it does not matter what type of a distribution function is employed. The situation is similar to the choice of a convenient representation in the conventional state-space approach for quantum mechanics.

§3.3. Wigner Phase Space Functions

In the preceding section a quantity C(t) known as a characteristic function was mentioned (3.2.5.) which was considered to be the fundamental quantity in terms of which a general distribution function is defined as

$$f(x) = \frac{1}{2\pi} \int dt C(t) \exp[-itx]$$

This section considers an explicit construction of such a distribution function appropriate to a quantum mechanical phase space where the random variables are generated by q-numbers $\hat{p}$, $\hat{q}$ taken to obey the commutation relations

$$\hat{p}\hat{q} - \hat{q}\hat{p} = \frac{\hbar}{i} \qquad (3.3.1.);$$

Therefore in terms of these variables the general distribution function is defined as

$$f(p,q) = \left(\frac{1}{2\pi}\right)^{2N} \int d\xi d\eta C(\xi,\eta) \exp[-i\xi\cdot p - i\eta\cdot q] \qquad (3.3.2.)$$

where the characteristic function

$$\begin{aligned} C(\xi,\eta) &= \langle \exp[i\xi\hat{p} + i\eta\hat{q}] \rangle \\ &= \langle \hat{C}(\xi,\eta) \rangle \\ &= \mathrm{Tr}[\hat{C}\,\hat{\rho}] \end{aligned} \qquad (3.3.3.)$$

Note that at this stage (3.3.3.) assumes nothing regarding the form of the characteristic function which remains indeterminate until we specify the relationship between $\hat{p}$ and $\hat{q}$ in order that the average in (3.3.3.) may be calculated. It becomes determined when we assume the commutation relations (3.3.1.) and the position representation of the momentum operator i.e.

$$p = \frac{\hbar}{i} \partial_q \qquad (3.3.4.)$$

since then the characteristic function may be evaluated using the complete set of wavefunctions $\{\psi_n(\tau)\}$ through (3.1.4.) as

$$C(\xi,\eta) = \sum_n P_n \int d\tau \psi_n^*(\tau) \exp[i\xi\hat{p} + i\eta\hat{q}]\psi_n(\tau) \qquad (3.3.5.)$$

$$= \sum_n P_n \int d\tau \psi_n^*(\tau) \exp[i\eta\hat{q}]\exp[i\xi\hat{p}]\psi_n(\tau)\exp[-i\xi\eta\hbar/2] \qquad (3.3.6.)$$

$$= \sum_n P_n \int d\tau \psi_n^*(\tau) \exp[i\eta\hat{q}]\psi_n(\tau + \hbar\xi)\exp[-i\xi\eta\hbar/2] \qquad (3.3.7.)$$

$$= \sum_n P_n \int d\tau \psi_n^*(\tau - \hbar\xi/2)\psi_n(\tau + \hbar\xi/2)\exp[i\eta\tau] \qquad (3.3.8.)$$

In going from (3.3.5.) to (3.3.6.) we have used the Baker-Hausdorff Lemma[96]:

$$\exp[\hat{A} + \hat{B}] \equiv \exp[\hat{A}]\exp[\hat{B}]\exp\tfrac{1}{2}[\hat{B},\hat{A}] \qquad (3.3.9.)$$

which holds whenever the operators $\hat{A}$ and $\hat{B}$ commute with their commutator i.e. whenever

$$[\hat{A},[\hat{A},\hat{B}]] = [\hat{B},[\hat{A},\hat{B}]] = 0 \qquad (3.3.10.)$$

(which of course they do in the case of operators $\hat{p}$, $\hat{q}$ since their commutator is just a constant (3.3.2.)). Also the transformation from (3.3.6.) to (3.3.7.) was performed utilising the translation property

$$\exp[a\partial x]f(x) = f(x + a) \qquad (3.3.11.)$$

If we now substitute this reduced form of the characteristic function (3.3.8.) into the general expression (3.3.2.) we obtain a particular distribution function:

$$f(p,q,t) = \left(\frac{1}{2\pi\hbar}\right)^{2N} \int d\xi d\eta \exp\left[\frac{-i\xi\cdot p}{\hbar} - \frac{i\eta\cdot q}{\hbar}\right] x$$

$$x \sum_n P_n \int d\tau \psi_n^*(\tau - \tfrac{\xi}{2},t)\psi_n(\tau + \tfrac{\xi}{2},t)\exp[i\eta\tau/\hbar]$$

which upon performing the τ-integration yields

$$f(p,q,t) = \left(\frac{1}{2\pi\hbar}\right)^N \int d\xi \sum_n P_n e^{-i\xi\cdot p/\hbar} \psi_n^*(q - \tfrac{\xi}{2},t)\psi_n(q + \tfrac{\xi}{2},t) \qquad (3.3.12.)$$

This particular expression of a quantum distribution function defined in terms of wavefunctions was first introduced for pure states in 1932 by Eugene Wigner[97] and has consequently become known as the Wigner distribution function. As can be seen from (3.3.12.) the Wigner distribution may be interpreted as a partial Fourier transform on the off diagonal elements of the density matrix.

The Wigner distribution has many useful properties, most of which are listed in Appendix I, but a few properties of direct interest may be extracted immediately from its' definition (3.3.12.). The first is that it is a real function since (3.3.12.) is invariant under taking its complex conjugate and changing variables $\xi \to -\xi$. Secondly integrating (3.3.12.) over p and q respectively shows that the projections of the Wigner function are just the usual position and momentum probability distributions so that it is normalised to unity. That is to say

$$\int dp f(p,q,t) = \sum_n P_n |\psi_n(q,t)|^2$$

$$\int dq f(p,q,t) = \sum_n P_n |\psi_n(p,t)|^2$$

and

$$\int dp dq f(p,q,t) = \sum_n P_n = 1$$

Therefore in the context of §3.2. we see that the Wigner distribution is both real and bounded and as a consequence of the Marcinkiewicz theorem we would generally expect it to assume negative values. This is indeed the case as an explicit example pertinent to an excited state of the harmonic oscillator shows in Appendix I.

Of course this negative-going behaviour of the Wigner distribution invalidates any direct interpretation of it as a probability function in the conventional sense. However we have already commented that a distribution function by itself should be regarded as a secondary quantity when compared

to its' use in calculating expectation values of observables through a prescription such as (3.1.7.) and so this peculiar (compared to classical mechanics) behaviour of the Wigner function should not be considered as detrimental.

In order to associate the calculation of averages with an integration over phase-space, we need not only the phase-space density as given here by the Wigner distribution, but also the phase-space function A(p,q) corresponding to the desired observable represented by the Hermitian operator $\hat{A}$ in state-space. We may obtain such a function by analogy with the construction of the Wigner distribution as follows.

We recognise in (3.3.2.) and (3.3.3.) that the Wigner distribution is associated with the particular density matrix of the system through a normalised Fourier transform, i.e.

$$f(p,q)\alpha \int d\xi d\eta \exp[-i\xi\cdot p - i\eta\cdot q]\mathrm{Tr}[\hat{C}\,\hat{\rho}]$$

where $\hat{C} = \exp[i\xi\hat{p} + i\eta\hat{q}]$. Consequently for a general Hermitian operator $\hat{A}$ we may associate a phase-space function A(p,q) by analogy with the above as:

$$A(p,q) = \text{const.} \int d\xi d\eta \exp[-i\xi\cdot p - i\eta\cdot q]\mathrm{Tr}[\hat{C}\hat{A}] \qquad (3.3.13.)$$

where the constant will be determined by requiring that the expectation of $\hat{A}$ may be given either in state-space or phase-space through

$$\langle\hat{A}\rangle = \mathrm{Tr}[\hat{A}\hat{\rho}] = \int dpdqA(pq)f(pqt) \qquad (3.3.14.)$$

If we substitute (3.3.2.) and (3.3.13.) into the phase-space average we find

$$\int dpdqA(pq)f(pq) = \frac{\text{const}}{(2\pi)^{2N}} \int d\xi d\eta d\xi' d\eta' dpdq \exp[-ip\cdot(\xi + \xi') - iq(\eta + \eta)]$$

$$\times \sum_{\substack{n,m \\ n',m'}} P_n \langle n|\hat{\rho}|m\rangle\langle m|\hat{C}(\xi,\eta)|n\rangle$$

$$\times \langle n'|\hat{A}|m'\rangle\langle m'|\hat{C}(\xi',\eta')|n'\rangle$$

$$= \text{const.} \int d\xi d\eta \sum_{\substack{n,m \\ n'm'}} P_n \langle n|\hat{\rho}|m\rangle\langle n'|\hat{A}|m'\rangle\langle m|\hat{C}(\xi,\eta)|n\rangle\langle m'|\hat{C}(-\xi,-\eta)|n\rangle \quad (3.3.15.)$$

If we consider the contribution to (3.3.15.) of the characteristic function matrix elements we find

$$\int d\epsilon d\eta \langle m|\hat{C}(\xi,\eta)|n\rangle\langle m'|\hat{C}(-\xi,-\eta)|n'\rangle$$

$$= \int d\xi d\eta d\tau d\tau' \exp[i\eta(\tau - \tau')]\psi^*_m(\tau - \hbar\xi/2)\psi_{n'}(\tau' - \hbar\xi/2)$$

$$\times \psi^*_{m'}(\tau' + \hbar\xi/2)\psi_n(\tau + \hbar\psi/2)$$

$$= (2\pi)^N \int d\xi \psi^*_{m'}(\xi)\psi_n(\xi) \int d\tau \psi^*_m(\tau)\psi_{n'}(\tau)$$

$$\equiv \left(\frac{2\pi}{\hbar}\right)^N \delta_{m',n}\delta_{m,n'}$$

which upon substituting back into (3.3.15.) gives

$$\int dpdqA(p,q)f(pq)$$

$$= \text{const.} \left(\frac{2\pi}{\hbar}\right)^N \sum_{n,m} P_n \langle n|\hat{\rho}|m\rangle\langle m|\hat{A}|n\rangle$$

$$= \text{const.} \left(\frac{2\pi}{\hbar}\right)^N \text{Tr}[\hat{\rho}\hat{A}] \quad (3.3.16.)$$

Therefore comparing (3.3.16.) with (3.3.14.) we see that if we define a phase-space function A(pq) corresponding to an arbitrary Hermitian operator $\hat{A}$ by:-

$$A(pq) = \left(\frac{\hbar}{2\pi}\right)^N \int d\xi d\eta \exp[-i\xi\cdot p - i\eta\cdot q]\text{Tr}[\hat{C}\hat{A}] \quad (3.3.17.)$$

then combined with the Wigner distribution function (3.3.12.) the average value of an observable (represented by either $\hat{A}$ or A(pq)) may be calculated either in state-space

$$\langle A\rangle = \text{Tr}[\hat{A}\rho]$$

or as a phase-space integration i.e.

$$\langle A \rangle = \int dpdqA(pq)f(pqt)$$

This final result is the principal appeal of using Wigner functions to study transport phenomena: with observable quantities represented in phase space by the Wigner equivalent of the operators (3.3.17.) and the phase-space density given by $(2\pi\hbar)^{-N}$ times the Wigner equivalent of the density matrix (3.3.12.), then transport calculations may be executed in direct analogy to classical mechanics. Therefore the differences between quantum and classical mechanics may be exhibited within a consistent descriptive framework, namely phase-space. The form of these differences will be manifest in two distinct ways: the first being due to the fact that in general the quantum phase-space observable A(pq) will have a different functional form to its' classical counterpart[54] (even if the latter exists) and the second aspect arises from the different behaviour of classical and quantum phase-space densities. Since the dynamical evolution of these distributions is governed by an equation of motion, the differences between classical and quantum dynamics should be inherent in the equations of motion. Therefore the primary aim in quantum transport theory should be to obtain an approximate equation of motion satisfied by the Wigner function which should exhibit effects explicitly due to the quantum nature of dynamical transport.

The next chapter illustrates perhaps the best method to date for obtaining an approximate transport equation under a given model situation.

CHAPTER 4

NON EQUILIBRIUM QUANTUM TRANSPORT THEORY

This chapter seeks to obtain suitable transport equations appropriate to describe non equilibrium electron/phonon processes due to strong externally applied fields in the medium-small-device. The philosophy followed assumes a basic model Hamiltonian which is then manipulated using sophisticated techniques borrowed from quantum field theory to obtain exact Greens functions equations. These same techniques are used to approximate the exact equations which may be interpreted in terms of the one-electron and one-phonon Wigner distribution functions.

Throughout this chapter the analysis is maintained as rigorous as possible bearing in mind that we would like to see physically meaningful equations at the end of it all. The rigour involved means that the chapter is both lengthy and complicated, but necessarily so since it is important to recognise the approximations we make in obtaining a description of nature where intuition based on previous experience can no longer be a guiding principle.

Where an approximation has been made to reduce the level of complexity an attempt is usually made to give an equivalent physical justification which, of course, will restrict the eventual transport theory to specific physical systems. The first major restriction occurs when we specify the model form of the Hamiltonian.

§4.1. The Model Hamiltonian

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§4.1. The Model Hamiltonian

The system we would like to describe is an interacting electron-electron-phonon assembly being driven by external electric and pressure fields for which we assume the Hamiltonian

$$H = \int d^3r\psi^\dagger(r)[\underset{(I)}{V(r)} - \frac{1}{2m}\underset{(II)}{\partial_{r_2}^2} + \frac{1}{2}\int \underset{(III)}{d^3r_2\psi^\dagger(r_2)\phi(r-r_2)\psi(r_2)}$$

$$+ \sum_k \underset{(IV)}{v_k e^{ik\cdot r} q_k}]\psi(r)$$

$$+ \frac{1}{2}\sum_k \underset{(V)}{(p_k^\dagger p_k + \Omega_k^2 q_k^\dagger q_k)} + \sum_k \underset{(VI)}{J_k q_k} \qquad (4.1.1.)$$

where the various terms labelled *(I)-(VI)* warrant some discussion.

The crystal ions are taken to vibrate simple harmonically about their equilibrium positions with a bare frequency of oscillation Ω_k. The q_k and p_k are the canonically conjugate co-ordinates and momenta describing the collective lattice vibrations which are related to the individual displacements q_i away from their equilibrium positions R_i^o by

$$q_i = i\sum_{k,\lambda}\sqrt{\frac{\hbar M}{2N\Omega_{k\lambda}}}\,\xi_{k,\lambda}e^{ik\cdot R_i^o}q_k \qquad (4.1.2.)$$

where λ is the number of atoms per unit cell, M the ion mass, N its' density, $\xi_{k\lambda}$ the polarisation vector and $\Omega_{k\lambda}$ the harmonic frequency.

Since the inter-ion interaction is expanded to second order in displacements only, the vibrational kinetic and potential energies are respectively $P^2/2$ and $\Omega^2q^2/2$ leading to the term *(V)* in the Hamiltonian. Anharmonic terms due to the phonon-phonon interaction are ignored, even though the theory would allow some scope to deal with them. This is because the phonon-phonon interaction would add even greater complications to an already complicated problem and these difficulties are not worth the compounded effort involved since although the model could not dissipate energy and thus give the correct equilibrium behaviour, we would not anticipate our short time scale dynamical systems to even reflect steady state results. As far as our situation is concerned, the prime intention is to examine processes directly involving the electrons and if necessary at a later point we could anticipate the role of the phonon-phonon

collisions by analogy with the electron-electron interactions.

We also allow for the possibility of an external field (J_k) capable of driving the phonons through the collective displacement amplitude q_k and hence the term *(VI)* in (4.1.1.). This field is taken to be non-electromagnetic in nature and so cannot drive the electrons out of equilibrium directly (although it may do so indirectly by the coupling through the electron-phonon interaction). For this reason we consider J to be the potential of an external pressure field.

The fourth term *(IV)* stems from taking the electron-ion interaction and Taylor expanding to the first non-trivial term (again an harmonic approximation) as follows. The potential on an electron at a place (r) due to the ion of sites R_j is just

$$\tilde{V}(r) = \sum_j V_{e-i}(r - R_j)$$

$$\simeq \sum_j V_{e-i}(r - R_j^o) + \sum_j q_j \cdot \nabla V_{e-i}(r - R_j^o)$$

which upon using (4.1.2.) becomes

$$V(r) = V^o(r) + \sum_k v_k e^{ik\cdot r} q_k \qquad (4.1.3.)$$

The first term in this expression represents the effect of the fixed periodic lattice on the electron which usually leads to the Bloch state description. However this term combines with the free electron kinetic energy $-\frac{1}{2m_o}\partial^2_{r^2}$, the sum of which is approximated by the effective mass form $-\frac{1}{2m}\partial^2_{r^2}$ given as the second term *(II)* in (4.1.1.) (that is to say the only effect of the fixed periodic lattice is to renormalise the free electron mass in this chapter. We are more directly concerned with dynamic renormalisation effects). The total electron-ion interaction is obtained by taking the second term in (4.1.3.) and integrating over the whole electron density which gives *(IV)* in (4.1.1.).

Of course the interaction magnitude v_k in (4.1.3.) depends on the bare phonon frequency Ω_k calculated in the harmonic approximation. Since the

interactions should alter this bare frequency we would also expect that the bare electron-ion interaction be normalised in some sense. However we do not introduce any such renormalisation at this stage but it will be calculated in a self-consistent fashion towards the end of this chapter. Because the model only permits one atom per unit cell and the phonons do not couple directly by electromagnetic interactions, we can assume that the electron-ion interaction considered represents a deformation potential coupling to acoustic phonons.

In a similar fashion we take the electrons to be driven by an external time-and space-dependent electric field $E(= -\nabla V(r,t))$ giving a total contribution represented by *(I)* in (4.1.1.). As already mentioned the phonons do not couple electromagnetically and so are not themselves driven directly by this external electric field although an indirect coupling through the electrons would exist. Both external electric and pressure fields are treated classically and it is assumed that the system cannot act back and interfere with the sources of these fields.

Finally, the third term *(III)* in (4.1.1.) is the potential energy due to the Coulombic electron-electron interaction which causes most of the problems in many body physics. It is worth pointing out here that unless it specifically states otherwise (as in §2.2. for example) this thesis always works in the Coulomb gauge. That is to say for an electromagnetic field with scalar (ϕ) and vector (A) potentials obeying the Maxwell source equation

$$\nabla^2\phi + \frac{1}{c}\,\partial_t\nabla\cdot A = -\rho(r) \qquad (4.1.4.)$$

then the Coulomb gauge demands that the vector potential satisfies $\nabla\cdot A = 0$ which from (4.1.4.) implies the scalar potential obeys

$$\nabla^2\phi(r,t) = -\rho(r,t) \qquad (4.1.5.)$$

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which has the solution

$$\phi(r,t) = \int d^3r' \frac{\rho(r',t)}{4\pi|r-r'|} \qquad (4.1.6.)$$

This represents the potential under the Coulomb gauge on a single electron at a place r. The total potential is obtained by integrating over the whole electron density giving rise to expression *(III)* in (4.1.1.).

It is important to recognise that this potential (4.1.6.) is instantaneous; moreover it is not an approximation but a consequence of using the Coulomb gauge (the Lorentz gauge and others would lead to retarded interactions. A discussion of the use of different gauges has already been given in §2.2.).

Finally, note the particular ordering of electron annihilation and creation operators in *(III)*: the $\psi^\dagger\psi^\dagger\psi\psi$ ordering is to ensure we do not consider an electron directly interacting with itself by virtual processes. These occur on an extremely fast time scale and so we take these and other similar very high frequency effects to act together to statically screen the Coulomb interaction. In other words the strength of the interaction is governed not by e^2 but by e^2/ϵ_∞ where ϵ_∞, the high frequency dielectric constant, is a medium dependent number due to the many very fast virtual transition processes.

In short, the model describes an interacting electron-electron-phonon system being driven by classical externally applied electric and pressure fields where the electrons interact electrostatically with each other and via the deformation potential with acoustic phonons.

§4.2. Exact Greens function equations of motion

This section seeks to obtain the equations of motion obeyed by the electron Greens function G(1,1') and the phonon correlation function D(1,1') {see Appendix II} under our model Hamiltonian (4.1.1.). Unless it is specifically included for clarity, we will work in units where $\hbar = 1$ so that Heisenbergs equation for the operator $\hat{O}$ (which refers to either the

electron annihilation operator $\psi(r_1,t_1)$ or the phonon displacement operator $q_{k_1}(t_1)$) is

$$i\partial_t \hat{O} = [\hat{O},H] \tag{4.2.1.}$$

Using the Hamiltonian (4.1.1.) in (4.2.1.) gives

$$\begin{aligned}[i\partial_{t_1} + \Delta_{r_1} - V(r_1t_1)]\psi(r_1,t_1) \\ = \sum_k v_k e^{ik\cdot r_1}\psi(r_1,t_1)q_k + \\ + \int d^3r_2\phi(r_1 - r_2)\psi^\dagger(r_2,t_1)\psi(r_2,t_1)\psi(r_1,t_1)\end{aligned} \tag{4.2.2.}$$

and

$$\begin{aligned}[\partial^2_{t_1} + \Omega^2_{k_1}]q_{k_1}(t_1) \\ = -v^*_{k_1}\int d^3r_2 e^{-ik_1\cdot r_2}\psi^\dagger(r_2,t_1)\psi(r_2,t_1) - J^*_{k_1}\end{aligned} \tag{4.2.3.}$$

where $\Delta_1 = \frac{1}{2m}\partial^2_{r_2}$ is the kinetic energy operator.

Using the definitions (II.4) and (II.16) we can convert (4.2.2.) and (4.2.3.) into equations of motion for the one-electron Greens function G(11') and the one-phonon correlation function D(1,1') respectively (recall from Appendix II that the shorthand co-ordinate notation (1,1') means (r_1,t_1, r_1',t_1') for the real space electron equations and $(k_1,t_1,k_1't_1')$ for the wavevector space of phonons. This should not lead to any confusion as the two equations will be considered seperately).

The resulting equations are

$$\begin{aligned}[i\partial_{t_1} + \Delta_1 - V(1)]G(1,1') \mp \int d2\phi(1 - 2)G_2(11'22^+) \\ -i\int d2v(1 - 2)\left[\frac{1}{i}\right]^2 <\hat{T}q(2)\psi(1)\psi^\dagger(1')> = \delta(1 - 1')\end{aligned} \tag{4.2.4.}$$

and

$$-[\partial_{t_1}^2 + \Omega_1^2]\, D(1,1')$$

$$- v^*(1)\left[\left(\frac{1}{i}\right)\langle \hat{T}q(1')\psi(1)\psi^\dagger(1^+)\rangle - Q(1')G(11^+)\right] = \delta(1-1') \qquad (4.2.5.)$$

The δ-function terms appear explicitly as we would expect in Greens function equations and arise from commuting the time ordering operator $\hat{T}$ with ∂_t since, for example

$$\begin{aligned}\partial_{t_1}[\hat{T}\psi(1)\psi^\dagger(1')] &\equiv \partial_{t_1}[\theta(t_1-t_1')\psi(1)\psi^\dagger(1') \pm \theta(t_1'-t_1')\psi^\dagger(1')\psi(1)] \\ &= \theta(t_1-t_1')\partial_{t_1}[\psi(1)\psi^\dagger(1')] \pm \theta(t_1'-t_1)\partial_{t_1}[\psi^\dagger(1')\psi(1)] \\ &+ [\psi(1)\psi^\dagger(1') \pm \psi^\dagger(1')\psi(1)]\delta(t_1-t_1') \\ &\equiv \hat{T}[\partial_{t_1}\{\psi(1)\psi^\dagger(1')\}] + \delta(1-1')\end{aligned}$$

or, rewriting

$$\begin{aligned}[\partial_{t_1}\hat{T} - \hat{T}\partial_{t_1}]\psi(1)\psi^\dagger(1') &= \delta(1-1') \\ &\equiv \delta(r_1 - r_1')\delta(t_1 - t_1') \qquad (4.2.6.)\end{aligned}$$

Thus the δ-function terms in the equations of motion (4.2.4.) and (4.2.5.) arises from changing $\hat{T}\partial_{t_1}$ with $\partial_{t_1}\hat{T}$. These equations also introduce the notation

$$\phi(1-2) \equiv \phi(r_1 - r_2)\delta(t_1 - t_2)$$

and similarly for $v(1-2)$.

It is clear that the one-particle Greens function equations depend on the two-particle Greens function and the mixed particle Greens function. Thus the coupled equations (4.2.4.) and (4.2.5.) represent the lowest members of the BBGKY hierarchy corresponding to the Hamiltonian (4.1.1.) (see §2.3.) which has no general closed solution. Therefore approximations have to be made which in general involve a truncation procedure by neglecting n-th order and higher correlations, an inherently inconsistent method as

discussed in §2.3. and Chapter 3. However the advantage of using multiple imaginary time Greens functions (Appendix II) is that these equations may be expressed[51] in a formally closed form without recourse to truncation techniques as follows.

If we take the Greens function in (4.2.4.) and (4.2.5.) to be expressed in the interaction picture in the imaginary time formalism (II.63) then the field dependence is contained solely in the S-matrix (II.64)

$$S = \exp[-i \int_0^{-i\beta} d2[V(2)n(2) + J(2)q(2)] \qquad (4.2.7.)$$

where we have taken the fields to be suddenly applied at time t = 0. In which case it is possible to functionally differentiate the one-particle Greens functions with respect to the electric and pressure fields seperately and in so doing, obtain formal identities between these functional derivatives and correlation functions. The procedure and relevant identities are derived in Appendix III where it is seen that it is possible to eliminate high order correlation functions in terms of function derivatives of lower order correlations. In particular we may use (III.6) - (III.9) to eliminate the two-electron Greens function and the mixed electron-phonon Greens functions from (4.2.4.) and (4.2.5.) to give

$$[i\partial_{t_1} + \Delta(1) - V(1)]G(11') \mp i \int d2\phi(1 - 2)[G(11')G(22^+) \pm \frac{\delta G(11')}{\delta V(2)}] - i \int d2v(1 - 2)[\frac{1}{i} Q(2)G(11') + \frac{\delta G(11')}{\delta J(2)}] = \delta(1 - 1') \qquad (4.2.8.)$$

and

$$-[\partial^2_{t_1} + \Omega^2_{k_1}]D(1,1') - iv^*_{k_1} \frac{\delta Q(1')}{\delta V(1)} = \delta(1 - 1') \qquad (4.2.9.)$$

However it is mathematically more convenient and indeed more appealing to recast (4.2.8.) into the form

$$[i\partial_{t_1} + \Delta_1 - V_{eff}(1)]G(11') - i\int d2\phi(1-2)\frac{\delta G(11')}{\delta V(2)} - i\int d2v(1-2)\frac{\delta G(11')}{\delta J(2)} = \delta(1-1') \qquad (4.2.10.)$$

where

$$V_{eff}(1) = V(1) \pm i\int d2\phi(1-2)G(22^+) + \int d2v(1-2)Q(2) \qquad (4.2.11.)$$

has the interpretation of an effective driving field on an electron which is composed of three parts: the external field, a mean field due to the contributions of all other electrons through the Coulomb potential and a mean field due to the distribution of lattice vibrations providing energy through the electron-phonon interaction strength. We can be a little more precise since we know from (II.6) that $G(2,2^+)$ is related to the local density of electrons $n(r_2,t_2)$ through

$$n(r_2,t_2) = \pm iG(2,2^+) \qquad (4.2.12.)$$

Therefore the electron contribution to the effective driving field is just

$$\int dr_2\phi(r_1 - r_2)n(r_2,t_1) \qquad (4.2.13.)$$

which is recognisable as the usual Hartree approximation to the effective potential on an electron[51][60][66][72]. Of course, (4.2.10.) is a physically more realistic way to express the equation of motion of an electron since the field actually driving the electron is not the external field, but a resultant field due to the intermediary influence of the medium in which the electron moves - in our case the interacting electrons and phonons would act to hinder the effects of a direct external field.

The important point to recognise concerning the equations (4.2.10.) and (4.2.9.) is that they involve only single particle quantities and the

functional derivatives of these quantities with respect to the driving fields. Of course this apparent closed nature is only formal since there are no general techniques for exactly solving functional derivative equations. To obtain recognisable transport equations it is still necessary to approximate the functional derivative and hence approximate the coupling to higher order correlation functions.

However writing the equations in this form at least allows some method of consistency in the method of approximation as we shall see in §4.7. Before we delve into this approximation scheme however, it is possible to proceed much of the way towards the final transport equations without having to specify the level of correlations we assume. This is illustrated in the next section when we consider the equation of motion of the one-electron Wigner distribution function.

§4.3. The general equation of motion for the one electron Wigner function

In the context of field theory the equations (4.2.9.) and (4.2.10.) are written in the form

$$[i\partial_{t_1} + \Delta_1 - V_{eff}(1)]G(11') - \int d\bar{1}\Sigma(1\bar{1})G(\bar{1}1') \qquad (4.3.1.)$$

$$-[\partial^2_{t_1^2} + \Omega^2_{k_1}]D(11') - \int d\bar{1}\Pi(1\bar{1})D(\bar{1}1') \qquad (4.3.2.)$$

which introduces the electron and phonon self energies respectively by

$$\Sigma(11') = -i\int d2d3\phi(1-2)G(13)\frac{\delta G^{-1}(31')}{\delta V(2)} - i\int d2d3v(1-2)G(13)\frac{\delta G^{-1}(31')}{\delta J(2)} \qquad (4.3.3.)$$

and

$$\Pi(11') = i\int d2d3d4v^*(1)G(13)\frac{\delta G^{-1}(34)}{\delta J(2)}G(41')D^{-1}(21') \qquad (4.3.4.)$$

where, to obtain (4.3.3.) and (4.3.4.) from (4.2.9.) and (4.2.10.) we have

used the definition of the inverse Greens function G^{-1} as

$$\int d\bar{1} G^{-1}(1\bar{1}) G(\bar{1}1') = \delta(1 - 1') \qquad (4.3.5.)$$

Thus all high order correlation effects are contained within the respective self energies which must eventually be approximated by using (4.3.3.) and (4.3.4.), although in this and the subsequent section we work with the general equations (4.3.1.) and (4.3.2.) leaving a specific determination until §4.7.

Henceforth in this section we are only concerned with the electron equation (4.3.1.) and its' counterpart:

$$[-i\partial_{t_1'} + \Delta_{1'} - V_{eff}(1')]G(11') - \int d\bar{1} G(1\bar{1}) \Sigma(\bar{1}1') = \delta(1 - 1') \qquad (4.3.6.)$$

These are imaginary time equations with no particular considerations of a specific time ordering. To obtain real time equations we must choose a particular ordering and analytically continue down the imaginary time axis onto the real axis while still maintaining the correct ordering of operators. In this particular situation the Greens functions are so defined that the analytic continuation is obtained simply by letting $-i\beta \to 0$. The resulting real time Greens functions are characterised by small letters, conforming to the notation of Kadanoff and Baym[50].

First then consider the particular time ordering $t_1 < t_1'$ in which case (4.3.1.) leads to

$$[i\partial_{t_1} + \Delta_1 - V_{eff}(1)]g^{<}(11') = \int_0^{t_1} d\bar{1}[\Sigma^{>}(1\bar{1}) - \Sigma^{<}(1\bar{1})]g^{<}(\bar{1}1') - \int_0^{t_1} d\bar{1}\, \Sigma^{<}(1\bar{1})[g^{>}(\bar{1}1') - g^{<}(\bar{1}1')] \qquad (4.3.7.)$$

and corresponding to (4.3.6.):

$$[-i\partial_{t_1'} + \Delta_{1'} - V_{eff}(1')]g^{<}(11') = \int_0^{t_1} d\bar{1}[g^{>}(1\bar{1}) - g^{<}(1\bar{1})]\Sigma^{<}(\bar{1}1') - \int_0^{t_1'} d\bar{1}g^{<}(1\bar{1})[\Sigma^{>}(\bar{1}1') - \Sigma^{<}(\bar{1}1')] \quad (4.3.8.)$$

(Recall from Appendix II that the notation "<" means the particular Greens function branch corresponding to $t_1 < t_1'$ and ">" refers to the other branch for $t_1 > t_1'$).

These two equations are combined to give a single equation for the real time ordered Greens function $g^{<}$ of

$$[i\partial_{t_1} + i\partial_{t_1'} + \Delta_1 - \Delta_{1'} - V_{eff}(1) + V_{eff}(1')]g^{<}(11') = \int_0^{t_1} d\bar{1}\{[\Sigma^{>}(1\bar{1}) - \Sigma^{<}(1\bar{1})]g^{<}(\bar{1}1') - [g^{>}(1\bar{1}) - g^{<}(1\bar{1})]\Sigma^{<}(\bar{1}1')\} - \int_0^{t_1'} d\bar{1}\{\Sigma^{<}(1\bar{1})[g^{>}(\bar{1}1') - g^{<}(\bar{1}1')] - g^{<}(1\bar{1})[\Sigma^{>}(\bar{1}1') - \Sigma^{<}(\bar{1}1')]\} \quad (4.3.9.)$$

In an identical fashion we arrive at the real time equation for the alternative time ordering of $t_1 > t_1'$ as:

$$[i\partial_{t_1} + i\partial_{t_1'} + \Delta_1 - \Delta_{1'} - V_{eff}(1) + V_{eff}(1')]g^{>}(11') = \int_0^{t_1} d\bar{1}\{[\Sigma^{>}(1\bar{1}) - \Sigma^{<}(1\bar{1})]g^{>}(\bar{1}1') - [g^{>}(1\bar{1}) - g^{<}(1\bar{1})]\Sigma^{>}(\bar{1}1')\} - \int_0^{t_1'} d\bar{1}\{\Sigma^{>}(1\bar{1})[g^{>}(\bar{1}1') - g^{<}(\bar{1}1')] - g^{>}(1\bar{1})[\Sigma^{>}(\bar{1}1') - \Sigma^{<}(\bar{1}1')]\} \quad (4.3.10.)$$

These last two equations form a basis from which manipulative techniques can be used to obtain a more physically appealing transport equation for the one-electron Wigner distributions as the remainder of this chapter aims to show.

The general philosophy is to somehow Wigner transform (Appendix II) the equations and then integrate over the (ω) variable to project out the Wigner distribution using the consistency condition (II.54). To this end we consider first the left hand side of equation (4.3.9.) which may be written in terms of the relative (r,t) and centre-of-mass (R,T) coordinates

by the transformations

$$r_1 \to R + \frac{r}{2} \quad r_1' \to R - \frac{r}{2}$$

$$t_1 \to T + \frac{t}{2} \quad t_1' \to T - \frac{t}{2}$$

as

$$[i\partial_T + \frac{1}{m}\partial_r\partial_R - V_{eff}(R + \frac{r}{2},T - \frac{t}{2}) + V_{eff}(R - \frac{r}{2},T + \frac{t}{2})]g^<(R,r,T,t) \quad (4.3.11.)$$

This equation may be Fourier transformed on the relative co-ordinates using (II.11) to give

$$-[\partial_T + \frac{P}{m}\cdot\partial_R]g^<(R,T,P,\omega) - DT \quad (4.3.12.)$$

where DT is the transform of the driving term given explicitly by

$$DT = \int d^3r dt e^{-iP\cdot r+i\omega t}[V_{eff}(R + \frac{r}{2},T - \frac{t}{2}) - V_{eff}(R - \frac{r}{2},T + \frac{t}{2})]g^<(R,r,T,t) \quad (4.3.13.)$$

To convert (4.3.12.) to an expression for the Wigner distribution function, from the consistency condition (II.54) i.e.

$$g^<(RTP\omega) = a(R,T,P,\omega)f(R,T,P)$$

and the sum rule for the spectral function (II.29.) i.e.

$$\int \frac{d\omega}{2\pi} a(R,T,P,\omega) = 1$$

we need to integrate (4.3.12.) over ω and divide by 2π which would give

$$-[\partial_T + \frac{P}{m}\cdot\partial_R]f(R,P,T) - \int \frac{d\omega}{2\pi} DT(\omega) \quad (4.3.14.)$$

This would have the appearance of the left hand side of the Boltzmann equation were it not for the troublesome non-local structure of the driving term (4.3.13.). However it is possible to express the third term in (4.3.13.) into a non-local differential form which corresponds closely

to the classically expected $F\cdot\partial f/\partial p$ structure. The expression (derived in Appendix IV) is:

$$\int \frac{d\omega}{2\pi} DT(\omega) = \frac{1}{\pi^3}\int d^3r'd^3k' \frac{\partial V_{eff}}{\partial r'}(R + r',T)ci[2k' r'] \frac{\partial f}{\partial k'}(P + k',R,T) \qquad (4.3.15.)$$

where $ci[x] = -\int_x^\infty dt\cos t/t$ is the cosine integral function[2].

This exact expression for the non-local driving term is discussed in Appendix IV where the following points are noted. It has aspects reminiscent of the usual semiclassical Boltzmann transport equation in that it depends on the driving field (the gradient of the potential) and the momentum derivative of the distribution function, but rather than being evaluated at a point (locally) they are displaced off the classical phase space trajectory with a weighting factor determined by the cosine integral function (non-locally).

The cosine integral function ensures that the dominant contribution to the sum comes from the classical trajectory but with a superimposed fringing structure as we integrate away from these local values.

It is possible to take the classical limit of (4.3.15.) (IV.10.) which yields the usual $F\cdot\partial f/\partial p$ structure. Later on we will introduce an approximation appropriate to the medium-small-device which reduces (4.3.15.) to the classical form, but for the present we will continue to work with the exact equation where the left hand side is determined from (4.3.14.) and (4.3.15.).

In a similar fashion we arrive at the corresponding left hand side of the equation for the other branch of the Greens function so that from (4.3.10.) we have

$$\int \frac{d\omega}{2\pi}[\partial_T + \frac{P}{m}\cdot\partial_R]g^>(RTP\omega) + \int \frac{d\omega}{2\pi} DT(\omega) \qquad (4.3.16.)$$

where the driving term is of the same form as (4.3.13.) but with $g^<$ replaced by $g^>$.

We now consider the structure of the collision integrals on the right hand sides of (4.3.9.) and (4.3.10.).

Specifically the right hand side of (4.3.9.) becomes, upon using the transformation $t_1 \to T - t/2$, $t_1' \to T + t/2$,

$$\begin{aligned} CI = &\int_0^T d\bar{1}\{\Sigma^>(1\bar{1})g^<(\bar{1}1') + g^<(1\bar{1})\Sigma^>(\bar{1}1') - g^>(1\bar{1})\Sigma^<(\bar{1}1') - \Sigma^<(1\bar{1})g^>(\bar{1}1')\} \\ &+ \int_T^{T-t/2} d\bar{1}\{[\Sigma^>(1\bar{1}) - \Sigma^<(1\bar{1})]g^<(\bar{1}1') - [g^>(1\bar{1}) - g^<(1\bar{1})]\Sigma^<(\bar{1}1')\} \\ &- \int_T^{T+t/2} d\bar{1}\{\Sigma^<(1\bar{1})[g^>(\bar{1}1') - g^<(\bar{1}1')] - g^<(1\bar{1})[\Sigma^>(\bar{1}1') - \Sigma^<(\bar{1}1')]\} \end{aligned} \tag{4.3.17.}$$

The only significant contribution to the collision integral of the electron Wigner distribution function comes from the first term in (4.3.17.). This is because when we Wigner transform and integrate over (ω) it is equivalent to inserting a $2\pi\delta(t)$ expression within the time integral and so the second two contributions in (4.3.17.) will be zero. Therefore the only relevant part to the collision integral we need to consider is

$$\begin{aligned} \int \frac{d\omega}{2\pi} CI(\omega) = \int d^3r e^{-iP\cdot r} \int_0^T d\bar{1}\{&\Sigma^>(1\bar{1})g^<(\bar{1}1') + g^<(1\bar{1})\Sigma^>(\bar{1}1') \\ &- \Sigma^<(1\bar{1})g^>(\bar{1}1') - g^>(1\bar{1})\Sigma^<(\bar{1}1')\}\Big|_{t_1 = t_1' = T} \end{aligned} \tag{4.3.18.}$$

Without loss of generality it is sufficient to manipulate the term

$$\int d^3r e^{-iP\cdot r} \int_0^T d\tau d^3\bar{r}\, \Sigma\,(r_1,\bar{r},T,\tau)g(\bar{r},r_1',\tau,T) \tag{4.3.19.}$$

Consider first the time integral in (4.3.19.)

i.e. $$\int_0^T d\tau\, \Sigma\,(T,\tau)g(\tau T)$$

which may be expanded in its' Fourier components as

$$\frac{1}{(2\pi)^4}\int_0^T d\tau \int d\omega' d\omega'' d\Omega' d\Omega'' \exp\left[i(\Omega' - \Omega'')(T - \tau) + i(\omega' + \omega'')\frac{(T + \tau)}{2}\right]$$

$$\times \sum (\Omega' + \frac{\omega'}{2}, \Omega' - \frac{\omega'}{2}) g(\Omega'' + \frac{\omega''}{2}, \Omega'' - \frac{\omega''}{2})$$

$$= \left(\frac{1}{2\pi}\right)^2 \int_0^T d\tau \int d\Omega' d\Omega'' \exp\left[i(\Omega' - \Omega'')(T - \tau)\right] \sum (\Omega, \frac{T + \tau}{2}) g(\Omega'', \frac{T + \tau}{2}) \qquad (4.3.20.)$$

where we have used the Wigner transform definition (II.11.).

Finally by changing variables the time integral part of (4.3.19.) becomes

$$\left(\frac{1}{2\pi}\right)^2 \int d\Omega' d\Omega'' \int_0^T d\tau 2e^{2i(\Omega' - \Omega'')(T-\tau)} \sum (\Omega', \tau) g(\Omega'', \tau) \qquad (4.3.21.)$$

The spatial integrals in (4.3.19.) follow a similar route. Explicitly:

$$\int d^3 r e^{-iP\cdot r} \int d^3\bar{r} \sum (\frac{r_1 + \bar{r}}{2}, r_1 - \bar{r}) g(\frac{r_1' + \bar{r}}{2}, \bar{r} - r_1') =$$

$$= \left(\frac{1}{2\pi}\right)^6 \int d\bar{r} dr dK' dK'' 2^3 e^{-2i(\bar{r}-R)(K'-K')} 2^3 e^{-2ir(P - \frac{K'+K''}{2})}$$

$$\times \sum (\bar{r} + \frac{r}{2}, K') g(\bar{r} - \frac{r}{2}, K'')$$

$$= \left(\frac{1}{2\pi}\right)^6 \int d\bar{r} dr dK dk 2^3 e^{2i(R-\bar{r})k} 2^3 e^{-2ir(P-K)}$$

$$\times \sum (\bar{r} + \frac{r}{2}, K + \frac{k}{2}) g(\bar{r} - \frac{r}{2}, K - \frac{k}{2}) \qquad (4.3.22.)$$

We recognise that (4.3.22.) is slightly more complicated than its' time analogue (4.3.21.) due to the fact that in the latter case we had integrated over (ω) which gave simpler results. We can now combine (4.3.22.) with (4.3.21.) into (4.3.18.) to give the resulting collision integral

$$\int \frac{d\omega}{2\pi} CI(\omega) = \left(\frac{1}{2\pi}\right)^8 \int dK dk d\bar{r} dr d\Omega' d\Omega'' \int_0^T d\tau$$

$$\times \{2^3 e^{2i(R-\bar{r})k} 2^3 e^{-2ir(P-K)} + c.c.\}\{2e^{2i(\Omega' - \Omega'')(T-\tau)} + c.c.\}$$

$$\times \{\sum^{>} (\bar{r} + \frac{r}{2}, K + \frac{k}{2}, \Omega', \tau) g^{<} (\bar{r} - \frac{r}{2}, K - \frac{k}{2}, \Omega'', \tau)$$

$$- \sum^{<} (\quad " \quad) g^{>} (\quad " \quad)\} \qquad (4.3.23.)$$

This is the collision integral corresponding to the equation for the Greens function branch $g^{<}(11')$. The collision integral corresponding to the alternative branch, $g^{>}(11')$ may be obtained from (4.3.23.) by the simple interchange of $g^{<} \leftrightarrow g^{>}$ and $\Sigma^{>} \leftrightarrow \Sigma^{<}$ combined with a complete sign change of the equation as can be seen by comparing the original equations (4.3.9.) and (4.3.10.). Therefore we may express the integrated real time Greens functions equations in the form

$$-\int \frac{d\omega}{2\pi} \{[\partial_T + \frac{P}{m} \partial_R] g^{<}(RTP\omega) + DT\} = \int \frac{d\omega}{2\pi} CI \qquad (4.3.24.)$$

$$+\int \frac{d\omega}{2\pi} \{[\partial_T + \frac{P}{m} \partial_R] g^{>}(RTP\omega) + DT\} = \int \frac{d\omega}{2\pi} CI \qquad (4.3.25.)$$

where $\int \frac{d\omega}{2\pi} DT$ is given in (4.3.15.) and $\int \frac{d\omega}{2\pi} CI$ in (4.3.23.).

Equation (4.3.24.) is readily transformed into an equation of motion for the electron Wigner distribution using (4.3.14.)(4.3.15.) and the consistency conditions (II.54.)(II.55.) to yield in detail

$$[\partial_T + \frac{P}{m} \partial_R] f(RPT) + \frac{1}{\pi^3} \int d^3r' d^3k' \frac{\partial V_{eff}}{\partial r'} (R + r', T) \frac{\partial f}{\partial k'} (P + k', R, T) ci[2k'r']$$

$$= -\frac{1}{(2\pi)^8} \int d^3k d^3K d^3\bar{r} d\Omega' d\Omega'' \int_0^T d\tau a(\bar{r} - \frac{r}{2}, \Omega'', \tau, K - \frac{k}{2})$$

$$\times \{2^3 e^{2i(R-\bar{r})k} + c.c.\} \{2e^{2i(\Omega'-\Omega'')(T-\tau)} + c.c.\}$$

$$\times \{\Sigma^{>}(\bar{r} + \frac{r}{2}, K + \frac{k}{2}, \Omega', \tau) f(\bar{r} - \frac{r}{2}, K - \frac{k}{2}, \tau)$$

$$- \Sigma^{<}(\quad " \quad)[1 - f(\quad " \quad)]\} \qquad (4.3.26.)$$

where $a(RTP\omega) \equiv g^{>}(RTP\omega) + g^{<}(RTP\omega)$ is the electron spectral function (II.24.).

This equation (4.3.26.) is the general equation of motion we wished to obtain for the one-electron Wigner distribution function. It is general in the sense that the self energy is as yet unspecified in terms of one particle Wigner distributions and so we have yet to approximate the dynamics of the collision processes. Moreover the electron spectral function appearing in this equation has also yet to be specified as this determines the allowed

energy distribution of the scattered non-equilibrium electron. In many respects the spectral function is the most important quantity in this equation and yet its general form is so complicated that drastic assumptions have to be made regarding its structure (indeed as we shall later on see the spectral function corresponds to the δ-function form of energy in the Fermi Golden Rule).

We will introduce an approximate form in terms of the electron self energy in §4.6. by using the physical assumption outlined in §4.5.

Without making any assumptions about the dynamics of the scattering events though, we may draw several inferences from this exact equation (4.3.26.). The first is that it is clearly structurally more complicated than the conventional Boltzmann approach would yield and yet it still maintains a sensible physical interpretation.

Our attention is immediately drawn to the non-local structure of this equation and particularly in the collision integral where we may impose the following interpretation.

Since the distinction between quantum and classical mechanics is embodied in the uncertainty relations we see that an instantaneous point collision in quantum mechanics is meaningless. If the precise position of a collision is unknown this will induce a spread in the possible momenta an electron may have after a collision and in the corresponding momentum of the scatterer. Similarly if the collision occurs on a finite time scale then the energies of electron and scatterer must remain uncertain. Therefore, given an electron with a specific momentum (if this were possible) then its' corresponding energy could be any one in a distribution of energies. The role of the spectral function is to supply this distribution and so is the quantum counterpart of the classical energy conserving δ-functions.

Consequently from the point of view of quantum mechanics we would expect the collision integral to be non local in space, time, momentum and

energy although its' precise form would have been difficult to guess.

A similar argument would lead us to expect that the driving term would also be non-local since even if the effective driving field acts instantaneously, then if the electron position is uncertain the driving field will act over this region (multiplied by a suitable weighting factor to allow for the increased probability of the electron lying in the centre of this range) and consequently should induce a spread in the momentum of the electron thereby leading to non-local integrals over momentum and position in the driving term. An additional comment on this term is that if the effective potential did not act instantaneously then we would also expect convoluted integrals over time and energy as well. Thus although we acknowledge the complicated structure of this equation, we recognise that the complications have physical origins in the extended nature of collisions being fundamentally limited by quantum mechanics.

In subsequent sections, (4.3.26.) will be reduced closer to a Boltzmann-like form under certain approximations, but before we consider these restrictions we first obtain a corresponding transport equation for the one-phonon Wigner distribution function.

§4.4. The general equation of motion for the one-phonon Wigner distribution

Much of the analysis of the preceding section may be used in obtaining an equation for the phonon Wigner distribution. However there are certain differences in this case due to the phonon correlation function (II.16.) being treated as the fundamental Greens function. Also because the phonons are essentially harmonic quasi-particles we find their equations are determined by second order time derivatives, in distinction to the electron case, as may be seen from (4.3.2.) and its' counterpart

$$-[\partial_{t_1}^2 + \Omega_{k_1}^2]D(11') - \int d\bar{1}\Pi(1\bar{1})D(\bar{1}1') = \delta(1 - 1') \qquad (4.4.1.)$$

$$-[\partial^2_{t_1} + \Omega^2_{K_1}]D(11') - \int d\bar{1}D(1\bar{1})\Pi(\bar{1}1') = \delta(1 - 1') \qquad (4.4.2.)$$

As a consequence of these second order time derivatives we note that the phonon self 'energy' $\Pi(11')$ given by (4.3.4.) has dimensions of $(\text{energy})^2$. This is why in the relationship between the phonon correlation function $D(RTK\omega)$ and the usual phonon Greens function $P(RTK\omega)$ given in (II.20.) we find an extra energy factor of $\hbar\omega_K$ i.e. explicitly from (II.20.):

$$D^{\gtrless}(RTK\omega) = \left(\frac{1}{2\hbar\omega_K}\right)[P^{\gtrless}(RTK\omega) + P^{\lessgtr}(RT - K - \omega)]$$

The reason why we choose to work with this correlation function rather than the phonon Greens function is because it is more natural. As we shall see it is mathematically more expedient to work with the correlations themselves, but also physically we can see from the model Hamiltonian (4.1.1.) that the electron scatters off the lattice wave displacement itself and so the prime quantity of interest should be a function connecting these displacements at different times and positions.

Consequently in this section we shall work with this correlation function, its' analytic branches and spectral function to a point where it is convenient to transfer over into phonon Greens functions $P^{\gtrless}$ and the corresponding spectral function using the connecting relationships obtained in Appendix II (II.20.) and (II.36.). From the phonon Greens functions we may then integrate over (ω) to project out the desired Wigner distributions from (II.56.).

Consider then the specific time ordering $t_1 < t_1'$ which from (4.4.1.) and (4.4.2.) gives

$$\begin{aligned}
&-[\partial^2_{t_1} - \partial^2_{t_1'}]D^<(11') - [\Omega^2_{K_1} D^<(11') - D^<(11')\Omega^2_{K_1'}] \\
&= \int_0^{t_1'} d\bar{1}\{[\pi^>(1\bar{1}) - \pi^<(1\bar{1})]D^<(\bar{1}1') - [D^>(1\bar{1}) - D^<(1\bar{1})]\pi^<(\bar{1}1')\} \\
&- \int_0^{t_1'} d\bar{1}\{\pi^<(1\bar{1})[D^>(\bar{1}1') - D^<(\bar{1}1')] - D^<(1\bar{1})[\pi^>(\bar{1}1') - \pi^<(\bar{1}1')]\}
\end{aligned} \qquad (4.4.3.)$$

We would now like to Wigner transform (4.4.3.) as in the electron case. Therefore if we just consider the left hand side for a moment, the first step is to change variables to relative and centre-of-mass co-ordinates which gives

$$\{2\partial_t\partial_T + [\Omega(K + \frac{k}{2}) + \Omega(K - \frac{k}{2})][\Omega(K + \frac{k}{2}) - \Omega(K - \frac{k}{2})]\}D^<(K,k,T,t) \qquad (4.4.4.)$$

The energy in this expression may be represented in a suggestive form if we Taylor expand to the lowest non-vanishing order about the centre-of-mass variables giving

$$[2\partial_t\partial_T + 2k\Omega_K\cdot\partial_K\Omega_K]D^<(K,k,T,t) \qquad (4.4.5.)$$

which may be Wigner transformed using the definition (II.11.):

$$D^<(R,T,K,\omega) = \int \frac{d^3k}{(2\pi)^3}\, dt e^{i\omega t + ik\cdot R}(i)D^<(K,k,T,t)$$

to give:

$$-2[\omega\partial_T + \Omega_K v_K\cdot\partial_R]D^<(R,T,K,\omega) \qquad (4.4.6.)$$

where the definition of the bare phonon group velocity has been introduced as

$$v_K = \partial_K\Omega_K \qquad (4.4.7.)$$

The content of the approximation that allowed a reduction of the non local form of the drift term in (4.4.4.) to the simple form given in (4.4.6.) will be known as the local-homogeneity-approximation when it is introduced more fully in §4.5. For the moment though we remark that $2\Omega_K v_K\cdot\partial_R D^<(RTK\omega)$ is the local approximation corresponding to the semi-classical limit of the exact non local expression:

$$-\frac{1}{(\pi\hbar)^3}\int d^3r'd^3k'\partial_{k'}\Omega^2(K+k')\partial_{r'}D^<(R+r',K,T,\omega)\mathrm{ci}[\frac{2k'r'}{\hbar}] \quad (4.4.8.)$$

which is derived in Appendix IV.

This exact form (4.4.8.) has the same convoluted non local structure as the electron case (4.3.13.) for the same reasons: since it is impossible to measure the wave amplitude of one specific position, the phonon correlation function must be averaged over some spread in position with a suitable weighting factor which depends on the momentum due to the uncertainty in the precise phonon frequency wavevector. Consequently the uncertainty principle leads us to expect integrals over position and momentum convoluted with some measure given to values relative to the classically expected ones which is of the content of (4.4.8.).

As already mentioned, the local homogeneity approximation which will be discussed later, reduces (4.4.8.) to a classical structure and due to the latters' simplicity when compared to the exact form we will continue to use (4.4.6.) in this section.

We can give this a reasonable justification because in this situation we see that the approximation amounts to neglecting second order derivatives (and higher) of the frequency with respect to its wavevector. In other words we are assuming that the bare phonon dispersion relation for Ω_K^2 is no more than quadratic which is certainly reasonable in the long wavelength limit since then it is equivalent to taking the velocity of sound to be constant. Of course this assumption only refers to the bare phonon frequency. The effects of electron-electron and electron-phonon interactions should act to modify the bare dispersion relationship and thus to assume the form (4.4.6.) does not detract from the dynamics of the problem with which we are concerned since the assumption does not refer to the renormalised dispersion relation.

Thus assuming (4.4.6.) and integrating over (ω) gives the desired Wigner equivalent of the left hand side of the original equation (4.4.3.) as

$$-2\int \frac{d\omega}{2\pi}[\omega\partial_T + \Omega_K v_K\cdot\partial_R]D^<(R,T,K,\omega) \qquad (4.4.9.)$$

Because the collision integrals on the right hand side of (4.4.3.) have an identical structure to the electron case considered in the last section the Wigner transform follows an identical procedure apart from a change in sign due to the differences in the definition (II.11.). Therefore by analogy with (4.3.23.) we may write down the Wigner transformed equivalent of the right hand side of (4.4.3.) as:

$$\int \frac{d\omega}{2\pi} CI_p(\omega) = \frac{-1}{(2\pi)^8}\int dK'dkd\Omega'd\Omega''drd\bar{r}\int_0^T d\tau$$

$$x\,[2^3 e^{2i(R-\bar{r})k}2^3 e^{-2ir(K-K')} + c.c.][2e^{2i(\Omega'-\Omega'')(T-\tau)} + c.c.]$$

$$\{\pi^>(\bar{r}+\frac{r}{2},K'+\frac{k}{2},\Omega',\tau)D^<(\bar{r}-\frac{r}{2},K'-\frac{k}{2},\Omega'',\tau)$$

$$-\ \pi^<(\quad''\quad)D^>(\quad''\quad)\} \qquad (4.4.10.)$$

which gives corresponding Wigner transformed equations for the phonon correlation functions:

$$2\int \frac{d\omega}{2\pi}[\omega\partial_T + \Omega_K v_K\partial_R]D^<(RTK\omega) = -\int \frac{d\omega}{2\pi} CI_p(\omega) \qquad (4.4.11.)$$

$$2\int \frac{d\omega}{2\pi}[\omega\partial_T + \Omega_K v_K\partial_R]D^>(RTK\omega) = -\int \frac{d\omega}{2\pi} CI_p(\omega) \qquad (4.4.12.)$$

It is now possible to transform (4.4.11.) into an equation for the phonon Greens function using the correspondence (II.20.) and restricting our attention to the positive (K,ω) part which easily yields

$$2\int \frac{d\omega}{2\pi}[\omega\partial_T + \Omega_K v_K\partial_R]P^<(RTK\omega) = -\int \frac{d\omega}{2\pi} CI_p(\omega)\Big|_{\substack{D^<\to P^< \\ D^>\to P^>}}$$

If we now use the consistency relation (II.56.) between $P^<$ and the one-phonon Wigner distribution n(RTK), combined with the sum rules satisfied by the phonon spectral function b(RTKω), i.e. from (II.32.) and (II.33.)

$$\int \frac{d\omega}{2\pi}\, b(RTK\omega) = 1$$

$$\int \frac{d\omega}{2\pi}\, \omega b(RTK\omega) = \omega_K$$

we can obtain an equation for the phonon Wigner distribution:

$$\begin{aligned}
&2[\omega_K \partial_T + \Omega_K v_K \cdot \partial_R] n(R,T,K) \\
&\quad = \left[\frac{1}{2\pi}\right]^8 \int dK' dk d\Omega' d\Omega'' dr d\bar{r} \int_0^T d\tau\, b\left(\bar{r} - \frac{r}{2}, K' - \frac{k}{2}, \Omega', \tau\right) \\
&\quad \times [2^3 e^{2i(R-\bar{r})k} 2^3 e^{-2ir(K-K')} + \text{c.c.}][2e^{2i(\Omega'-\Omega'')(T-\tau)} + \text{c.c.}] \\
&\quad \times \{\pi^>\left(\bar{r} + \frac{r}{2}, K' + \frac{k}{2}, \Omega', \tau\right) n\left(\bar{r} - \frac{r}{2}, K' - \frac{k}{2}, \tau\right) \\
&\quad - \pi^<(\quad " \quad)[1 + n(\quad " \quad)]\}
\end{aligned} \tag{4.4.13.}$$

This is the general equation for the phonon Wigner distribution function accompanying the electron equation obtained in the last section (4.3.26.). It has all the same non-local structure in the collision integral and, had we not approximated (4.4.8.) with a Taylor expansion it would also have had non-local structure in the diffusion term.

We have yet to specify a form for the phonon spectral function b(RTKω), the phonon self energy π(RTKω) and the renormalised phonon frequency ω_K which is <u>not</u> the same as the bare frequency Ω_K since it stems from the commutation relations between the phonon annihilation operator and the <u>total</u> Hamiltonian (see (II.34.)). We may also see from (4.4.13.) that the renormalised phonon frequency has the effect of renormalising the phonon group velocity to

$$\bar{v}_K = \frac{\Omega_K}{\omega_K} \partial_K \Omega_K \qquad (4.4.14.)$$

Thus to summarise the last two sections, we have obtained general quantum transport equations for the one-electron and one-phonon Wigner distributions appropriate to a model Hamiltonian (4.1.1.). These equations are structurally different to the conventional Boltzmann transport equations and yet still maintain the possibility of physical interpretation even in their general form. The most striking difference is the convoluted non-local structure occuring in the collision integrals and driving terms as a consequence of the quantum nature of transport: the particle wavepackets as represented by Wigner distributions have a dispersion away from the classical values and as such interact over a range in phase-space. Since the collisions are non point-like, the correlations from one collision will not have died away by the time the next collision occurs. Therefore the particles are always in non-stationary states which is why the upper time integral limit cannot be extended to infinity as in Boltzmann transport (at which time the carrier is considered to have settled into a stationary state). Consequently the equations are time reversible as may be explicitly seen by changing $t \to -t$ and $P \to -P$. This may be interpreted as the correlations from one collision being carried through to subsequent events, an effect often refered to in the literature as the carrier retaining a memory of its' past history. A further consequence of not using an asymptotic time integral is that by the uncertainty relations we can not therefore specify precisely a carriers energy but only the distribution of possible energies. This accounts for the appearance of electron and phonon spectral functions replacing the more usual δ-function of the Boltzmann transport theory.

However the equations (4.3.26.) and (4.4.13.) are obviously too general to be of any practical use in specific problems as we have yet to specify the self energies and spectral functions. This is impossible to

do exactly and so we must resort to approximations which are simple but sufficiently restrictive to ensure they still apply to physical systems.

In our particular situation where we would like to model the medium-small-device as the transition from the semi-classical to completely quantum transport we would hope that the time and space scales characterizing the system are sufficiently large compared to the corresponding scales characterizing the particles so that we are able to assume microscopically smooth variations which would lead to a simplification in the description of the resulting transport. The approximation that this assumption leads to is termed the local-homogeneity-approximation.

§4.5. The Local Homogeneity Approximation

In the previous section an approximation was made in simplifying the phonon diffusion term to obtain a classical-like expression which amounted to a Taylor expansion to lowest non-vanishing order about the centre-of-mass variables. The assumptions behind this approximation can be used to reduce the general quantum transport equations to a slightly simpler form and indeed will be used in subsequent sections to obtain approximate expressions for the self energies and spectral functions.

We may introduce the approximation most directly by considering the general equation of motion for the one-electron Wigner distribution:

$$[i\partial_{t_1} - i\partial_{t_1'} + \frac{1}{2m}\partial^2_{r_1} + \frac{1}{2m}\partial^2_{r_1'}]G(11') - \int d2[\Sigma(12)G(21') + G(12)\Sigma(21')] = 2\delta(1-1') \quad (4.5.1.)$$

or equivalently in the relative and centre-of-mass co-ordinates,

$$[2i\partial_t + \frac{1}{2m}(2\partial^2_R + \frac{1}{2}\partial^2_r)]G(R,T,r,t) - \int dr_2 dt_2 [\Sigma(R + \frac{r_2}{2}, r - r_2, T + \frac{t_2}{2}, t - t_2)G(R + \frac{r_2 - r}{2}, r_2, T + \frac{t_2 - t}{2}, t_2) + G(\quad " \quad)\Sigma(\quad " \quad)] = 2\delta(t)\delta(r) \quad (4.5.2.)$$

We would now like to Fourier-Laplace transform this equation on the relative co-ordinates but because it is not of a simple convoluted integral structure, it does not have a simple transform. The local-homogeneity-approximation assumes that a simple transform is a reasonably accurate representation of the physics within the following assumptions.

The variables (R,T,P,Ω) of the Greens functions may be considered to represent a point in an eight dimensional phase-space. Classically, as T increases the parameters (R,P,Ω) would continuously evolve and the sequence of parameters $(R(T),P(T),\Omega(T))$ identify a trajectory in this phase-space on which all quantities are evaluated. As we have already noted, from a quantum mechanical viewpoint we would expect a dispersion away from the classical trajectory and so the evaluation of quantities would not only depend on the classical trajectory but also must be weighted with contributions away from this particular phase-space path.

Therefore a first approximation would be to assume the weighting given to values on the classical trajectory be so great that we may reasonably neglect contributions from all the 'off-path' variables thus leading to a semiclassical picture. We are therefore assuming that the alternating signs of the cosine integral function (Fig. IV.1.) act to smooth out the non-local structure completely leaving the dominant contribution from the local classical trajectory.

This assumption is then easily used to obtain a simple transform of (4.5.2.) since if we consider the term

$$\int dr_2 dt_2 \int dr dt e^{-iP\cdot r+i\Omega t} \sum\left(R + \frac{r_2}{2}, r - r_2, T + \frac{t_2}{2}, t - t_2\right) \times G\left(R + \frac{r_2 - r}{2}, r_2, T + \frac{t_2 - t}{2}, t_2\right) \qquad (4.5.3.)$$

and then neglect the contributions evaluated off the classical trajectory determined by the centre-of-mass co-ordinates then it reduces to the form

$$\int drdte^{-iP\cdot r+i\Omega t}\int dr_2dt_2\sum(R,r-r_2,T,t-t_2)G(R,r_2,T,t_2)$$

$$=\sum(RTP\Omega)G(RTP\Omega) \qquad (4.5.4.)$$

Therefore using (4.5.4.) the equation of motion (4.5.2.) may be Wigner transformed under the local-homogeneity-approximation to give

$$\left(\omega-\frac{P^2}{2m}\right)G(RTP\omega)-\sum(RTP\omega)G(RTP\omega)=1$$

or

$$G(RTP\omega)=1/[\omega-\varepsilon(P)-\sum(RTP\omega)] \qquad (4.5.5.)$$

(This approximation for the electron Greens function will be used in the next section to obtain an expression for the electron spectral function).

Similarly we may take the general phonon correlation function equation:

$$-[\partial_{t_1}^2+\partial_{t_1'}^2+\Omega_{k_1}^2+\Omega_{k_1'}^2]D(11')-\int d\bar{1}[\pi(1\bar{1})D(\bar{1}1')+$$

$$+D(1\bar{1})\pi(\bar{1}1')]=2\delta(1-1') \qquad (4.5.6.)$$

and Wigner transform under the local-homogeneity-approximation to obtain the phonon correlation function in the form

$$D(RTK\omega)=1/[\omega^2-\Omega_K^2-\pi(RTK\omega)] \qquad (4.5.7.)$$

It is evident from (4.5.3.) and (4.5.4.) that the local-homogeneity-approximation is equivalent to a Taylor series expansion about the classical trajectory to lowest non-vanishing order. This gives an alternative viewpoint of the local-homogeneity-approximation in that it demonstrates that the self energy is assumed to be slowly varying in the sense that the Taylor expansion requires

$$\frac{R}{\Sigma(R)}\frac{\partial\Sigma}{\partial R}\ll 1 \qquad (4.5.8.)$$

For the self energy to be interpreted as a slowly varying function

we are implicitly assuming the system is macroscopic when compared to the scales on which disturbances occur such as mean collision lengths and durations.

We can thus use the local-homogeneity-approximation to simplify the general equations of motion of the electron and phonon Wigner distributions.

First consider the non-local electron driving term (4.3.15.) i.e.

$$\frac{1}{\pi^3}\int d^3r'd^3k' \frac{\partial V_{eff}}{\partial r'}(R + r',T)\frac{\partial f}{\partial k'}(P + k',R,T)Ci[2k'\cdot r'] \quad (4.5.9.)$$

Under the local homogeneity-approximation the driving field is only evaluated on the classical trajectory which introduces a representation of a δ-function through the cosine integral. Thus (4.5.9.) collapses to the form

$$-\partial_R V_{eff}(R,T)\partial_P f(R,P,T) \quad (4.5.10.)$$

which is just the usual classical driving term as we expect since we are only concerned with the local expressions evaluated on the centre of mass trajectory which is a semi-classical approximation.

Similarly the collision integral may be greatly simplified by changing variables on the right hand side of (4.3.26.) which becomes

$$\begin{aligned}-\left(\frac{1}{2\pi}\right)^8 \int_0^T & d\tau d\Omega' d\Omega'' dk dK dr d\bar{r} a(R - \bar{r} - \tfrac{r}{2}, P - K - \tfrac{k}{2}, \Omega'', T - \tau) \\ & \times \{2^3 e^{2ir\bar{k}} 2^3 e^{-2irK} + c.c.\}\{2e^{2i(\Omega'-\Omega'')\tau} + c.c.\} \\ & \times [\sum^{>}(R - \bar{r} + \tfrac{r}{2}, P - K + \tfrac{k}{2}, \Omega', T - \tau) f(R - \bar{r} - \tfrac{r}{2}, P - K - \tfrac{k}{2}, T - \tau)] \\ & - \sum^{<}(\quad " \quad)[1 - f(\quad " \quad)] \end{aligned} \quad (4.5.11.)$$

By assuming the self energy, spectral function and distribution function are to be evaluated on the classical trajectory this collision integral may be contracted to

$$\frac{-1}{(2\pi)^2}\int d\Omega' d\Omega'' \int_0^T d\tau\{2e^{2i(\Omega'-\Omega'')(T-\tau)} + c.c.\}a(R,P,\Omega'',\tau)$$
$$x\,[\sum^{>}(R,P,\Omega',\tau)f(R,P,\tau) - \sum^{<}(RP\Omega'\tau)\{1 - f(RP\tau)\}] \qquad (4.5.12.)$$

An identical procedure reduces the phonon collision term to a similar form to (4.5.12.) and the phonon drift term has already been reduced to semi-classical form by using the local-homogeneity-approximation in the previous section. Therefore the resulting equations of motion for the electron and phonon Wigner distributions under the local-homogeneity-approximation may be written down in full as :-

$$[\partial_T + \frac{P}{m}\cdot\partial_R + F(R,T)\cdot\partial_p]f(R,P,T)$$
$$= -\left(\frac{1}{2\pi}\right)^2 \int d\Omega' d\Omega'' \int_0^T d\tau\{2e^{2i(\Omega'-\Omega'')(T-\tau)} + c.c.\}a(R,P,\Omega'',\tau)$$
$$x\,\{\sum^{>}(RP\tau\Omega')f(R,P,\tau) - \sum^{<}(RP\tau\Omega')[1 - f(RP\tau)]\} \qquad (4.5.13.)$$

$$[\partial_T + \bar{v}_K\cdot\partial_R]n(R,T,K)$$
$$= \left(\frac{1}{2\pi}\right)^2 \int d\Omega' d\Omega'' \int_0^T d\tau\{2e^{2i(\Omega'-\Omega')(T-\tau)} + c.c.\}\frac{b(R,K,\Omega'',\tau)}{2\omega_K}$$
$$x\,\{\pi^{>}(RK\tau\Omega'')n(R,K,\tau) - \pi^{<}(RK\tau\Omega'')[1 + n(R,K,\tau)]\} \qquad (4.5.14.)$$

where $F(R,T) = -\partial_R V_{eff}(R,T)$, ω_K is the renormalised phonon frequency and $\bar{v}_K$ is the renormalised phonon group-velocity (4.4.14.).

The use of the local-homogeneity-approximation is perhaps the most drastic assumption made in this thesis in that it reduces very complicated quantum transport equations into almost classical equations as exhibited in the above equations (4.5.13.) and (4.5.14.), with a remaining significant difference contained in the finite (non-asymptotic) time integral.

This is an important point often overlooked in transport theories. The boundary conditions are specified at T = 0 at which time a field is <u>suddenly</u> applied driving the system out of equilibrium: there is no ficticious adiabatic turning on of the fields and interactions and asymptotic

descriptions of scattering through steady states. Instead it is important to deal with finite time intervals which of course precludes only δ-function form of energy conserving factors.

This is particularly important in the medium small device where although semi-classical concepts may still be valid, the transit time of carriers from source to drain is comparable to the relaxation times in the device thus ruling out any physical description in terms of steady states and asymptotic functions.

One final comment on this pair of equations is that even though the self energies and spectral functions have yet to be determined (under the local homogeneity approximation), we can already see a quasi-particle description of the transport emerging through the effective driving fields and renormalised phonon frequencies and group velocities.

§4.6. The electron and phonon spectral functions

In Appendix II, the electron and phonon spectral functions were defined and explicitly evaluated under non-interacting conditions, in which case they are singular δ-functions - each value of momentum uniquely determines the electrons energy and each wavevector value specifies one phonon frequency. This section seeks to obtain approximate expressions for the spectral functions under interacting circumstances complicated by effective driving fields.

Apart from the non-interacting case, it is impossible to obtain exact forms for these spectral functions since the interactions make this a complicated many body problem. Moreover, if we did have an exact algebraic expression then we would also know the corresponding Greens function exactly and hence the Wigner distribution and thus knowing the distribution function we would have no need for a transport equation. Therefore we can understand that by introducing interactions, the best we can hope for is to obtain a spectral function that depends on the Wigner distribution itself and so

introducing a self-consistent scheme.

To this end we begin by considering an equilibrium situation in an homogeneous medium where we allow for interactions. Because the equilibrium system is homogeneous, the Greens functions and self energies depend only on the co-ordinate differences $r_1 - r_1'$ and $t_1 - t_1'$ so that the electron equation of motion

$$[i\partial_{t_1} + \frac{1}{2m}\partial^2_{r_1}]G(1 - 1') - \int d\bar{1}\sum(1 - \bar{1})G(\bar{1} - 1') = \delta(1 - \bar{1}') \quad (4.6.1.)$$

may be simply Wigner transformed to give

$$G(P,\omega) = 1/[\omega - \varepsilon(P) - \sum(P,\omega)] \quad (4.6.2.)$$

where $\varepsilon(P) = P^2/2m$ is the electrons kinetic energy.

The self energy $\sum$ is itself a Greens function and thus may be expressed in terms of its' spectral function Γ by (c.f. (II.27.))

$$\sum(P,\omega) = \int \frac{d\omega'}{2\pi} \frac{\Gamma(P,\omega)}{\omega - \omega'} \quad (4.6.3.)$$

We can thus use (4.6.2.) and (4.6.3.) to express the electron spectral function in terms of the real and imaginary parts of the self energy since from the definition (II.28.):

$$\begin{aligned} A(P,\omega) &= i[G(P,\omega + i\delta) - G(P,\omega - i\delta)] \\ &= \frac{\Gamma(P,\omega) + \delta}{[\omega - \bar{\varepsilon}(P,\omega)]^2 + [\frac{\Gamma(P,\omega) + \delta}{2}]^2} \end{aligned} \quad (4.6.4.)$$

where it is understood that the expression is evaluated in the limit of $\delta \to 0$. We have made use of the fact

$$\begin{aligned} \sum(P,\omega \pm i\delta) &\equiv \int \frac{d\omega'}{2\pi} \frac{\Gamma(P,\omega')}{\omega - \omega' \pm i\delta} \\ &= P\int \frac{d\omega'}{2\pi} \frac{\Gamma(P,\omega')}{\omega - \omega' \pm i\delta} \mp \frac{i}{2}\Gamma(P,\omega) \end{aligned} \quad (4.6.5.)$$

so that the energy $\bar{\varepsilon}(P,\omega)$ in (4.6.4.) is an effective electron energy

including contributions from the real part of the electron self energy, explicitly:

$$\bar{\varepsilon}(P,\omega) = \varepsilon(P) + \mathrm{Re}\sum(P,\omega) = \varepsilon(P) + P\int \frac{d\omega'}{2\pi}\frac{\Gamma(P,\omega')}{\omega - \omega'} \qquad (4.6.6.)$$

It is interesting that if the imaginary part of the self energy is non zero then the spectral function (4.6.4.) has the form of a Lorentzian distribution of width Γ, the peak value of which occurs at $\omega = \bar{\varepsilon}$ as opposed to $\omega = \varepsilon(P)$ if we had a non-interacting system. In the limit of this imaginary part of the self energy tending to zero, the spectral function collapses to a singular δ-function of argument $\omega - \bar{\varepsilon}$ and thus we see that the effect of interactions is to broaden and shift the energy conserving factors which in the Fermi-Golden-Rule approach would be determined by δ-functions.

Before we proceed, it is useful to consider the form of the spectral function in the Hartree-Fock approximation to the electron gas problem. In general the one electron equation would be of the form

$$[i\partial_{t_1} + \frac{1}{2m}\partial^2_{r_1}]G(11') \mp i\int d2\phi(1-2)G_2(11'22^+) = \delta(1-1') \qquad (4.6.7.)$$

In the Hartree approximation we assume that the two electron Greens function is a product of two one-electron Greens functions so that the self energy in the Hartree approximation is just

$$\sum(11') = \delta(1-1')\int d2\phi(1-2)\langle n(2)\rangle \qquad (4.6.8.)$$

where we have compared with (4.6.1.). For a homogeneous system the local electron density is independent of position and so $\langle n(r_2)\rangle = n = \text{constant}$. Therefore

$$\sum(P,t) = n\langle\phi\rangle\delta(t) \qquad (4.6.9.)$$

where we have introduced the average energy contributed by the Coulomb potential as $\langle\phi\rangle \equiv \int dr\phi(r)$.

Thus from (4.6.9.) the Hartree self energy as a function of ω is constant i.e.

$$\sum(P,\omega) = n\langle\phi\rangle \qquad (4.6.10.)$$

and therefore it must be a real function. Consequently the electron spectral function in this case, from (4.6.4.), is just a δ-function i.e.

$$A_H(P) = 2\pi\delta(\omega - \varepsilon_H(P)) \qquad (4.6.11.)$$

where $\varepsilon_H(P) \equiv \varepsilon(P) + n\langle\phi\rangle$ is the effective Hartree energy which includes the mean contribution from the surrounding electron density.

The Hartree-Fock approximation expands this approach by taking into account exchange effects as simply as possible so that the two electron Greens function is assumed of the form

$$G_2(11'22^+) = G(11')G(22^+) \pm G(12^+)G(21') \qquad (4.6.12.)$$

In this case the electron self energy is given by

$$\sum(11') = \delta(1 - 1')\int d2\phi(1 - 2)\langle n(2)\rangle + i\phi(1 - 1')G(11') \qquad (4.6.13.)$$

which, in a homogeneous medium is just

$$\sum(1 - 1') = n\langle\phi\rangle\delta(1 - 1') + i\phi(1 - 1')G(1 - 1') \qquad (4.6.14.)$$

which is easily transformed to give a self energy as a function of momentum to be purely real again (and thus independent of ω) i.e.

$$\sum_{HF}(P) = n\langle\phi\rangle \pm \int \frac{d^3P'}{(2\pi)^3}\phi(P - P')\langle\hat{n}(P')\rangle \qquad (4.6.15.)$$

Therefore the corresponding spectral function is again a δ-function but now it depends on the effective Hartree-Fock energy

$$\varepsilon_{HF}(P) = \varepsilon(P) + n\langle\phi\rangle \pm \int \frac{d^3P'}{(2\pi)^3}\phi(P - P')\langle\hat{n}(P')\rangle \qquad (4.6.16.)$$

In both these instances the approximations assume that the electrons move as free particles in a mean potential produced by the surrounding electron

density.

It is straightforward to see that this δ-function form of the spectral function is achieved whenever the self energy has no frequency component, or in other words whenever

$$\Sigma(r_1 - r_1', t_1 - t_1') \equiv \Sigma(r_1 - r_1')\delta(t_1 - t_1')$$

In the specific case considered here, this is a direct consequence of the Coulomb interaction being instantaneous in time. This is an important point because we know that many body effects will act to shield out the bare Coulomb interaction and in a dynamic situation where the shielding is not instantaneous due to the finite velocity and hence finite response time of the electron density, the shielded potential will be retarded in time. This will induce an imaginary component in the self energy which will become frequency dependent leading to a spread in the spectral function which will be illustrated in §4.7.

If the system is not strictly homogeneous but we may assume that the spatial variations are still slow, then we would anticipate that the self energy becomes a function of (R,T) as well as (P,ω) and that the spectral function would be of the form

$$A(R,T,P,\omega) = \frac{\Gamma(R,T,P,\omega) + \delta}{[\omega - \bar{\varepsilon}(RTP\omega)]^2 + [\frac{\Gamma(RTP\omega) + \delta}{2}]^2} \quad (4.6.17.)$$

In fact this is precisely the result we obtain under the local-homogeneity-approximation since if we use the previously obtained Greens function (4.5.5.) in the definition (II.28.) we end up with the result (4.6.17.). Therefore this is the form of the spectral function defined in terms of the electron self energy under the local-homogeneity-approximation we require.

In a similar manner we may use the phonon correlation function given under the local-homogeneity approximation by (4.5.7.) to obtain an expression

for its' spectral function in the definition (II.35.) as:

$$S_D(RTK\omega) \equiv i[D(R,T,K,\omega + i\delta) - D(R,T,K,\omega - i\delta)]$$

$$= i\left\{\frac{1}{\omega^2 - \omega_K^2 + i\,\frac{\gamma(RTK\omega)}{2} + i\delta}\right.$$

$$\left. - \frac{1}{\omega^2 - \omega_K^2 + i\,\frac{\gamma(R,T,\omega - K, - \omega)}{2} - i\delta}\right\} \qquad (4.6.18.)$$

where we have used the definition of the phonon self energy π in terms of its' spectral function γ as

$$\pi(R,T,K,\omega) = \int \frac{d\omega'}{2\pi}\,\frac{\gamma(R,T,K,\omega')}{\omega - \omega'} \qquad (4.6.19.)$$

and where we have also used the fact that $\gamma(R,T,K,\omega) = -\gamma(R,T, - K, - \omega)$ which follows since $S_D(RTK\omega)$ is an odd function of (K,ω) as may be seen from its' definition (II.36.).

We also note that (4.6.18.) is expressed in terms of a renormalised frequency ω_K instead of the bare frequency Ω_K which is defined in terms of the real part of the self energy as

$$\omega_K^2 \equiv \Omega_K^2 + Re\pi(R,T,K,\omega) \qquad (4.6.20.)$$

Therefore in the same manner that interactions alter the electrons peak energy through the self energy (4.6.6.), the bare phonon frequency is similarly altered to the renormalised frequency ω_K determined through (4.6.20.) as a consequence of the interactions between electrons and phonons.

This is the renormalised frequency that appears in the phonon Wigner distribution equation of motion (4.5.15.) which also acts to produce a renormalised group velocity (4.4.14.).

If we continue in the spirit of the quasi-particle approximation and assume that the lifetime (defined as the inverse of the imaginary part of the self energy) of this renormalised phonon is sufficiently long so that the imaginary part is much smaller than the real part of the self energy,

then the expression for the spectral function (4.6.18) approximates to

$$S_D(R,T,K,\omega) = i\left\{\frac{1}{[\omega + i\frac{\gamma(R,T,K,\omega)}{4\omega}]^2 - \omega_K^2} - \frac{1}{[\omega + i\frac{\gamma(R,T,-K,-\omega)}{4\omega}]^2 - \omega_{-K}^2}\right\} \qquad (4.6.21.)$$

which may be rearranged in the form

$$S_D(R,T,K,\omega) = \frac{1}{2\omega_K}[B(R,T,K,\omega) - B(R,T,-K,-\omega)]$$

where

$$B(R,T,K,\omega) = \frac{\alpha(R,T,K,\omega)}{[\omega - \omega_K]^2 + [\frac{\alpha(R,T,K,\omega)}{2}]^2} \qquad (4.6.22.)$$

and $\alpha(R,T,K,\omega) \equiv \frac{\gamma(R,T,K,\omega)}{2\omega}$ has the dimensions of energy and may be regarded as the spectral function of the phonon Greens function P(RTKω) (II.14.) since from (II.36.), B(R,T,K,ω) may be interpreted as its' spectral function.

Similar to the electron case we see that in the limit of $\alpha \to 0$ the true phonon spectral function (4.6.22.) reduces to the usual δ-function form generally used in discussions of phonon transport[72], i.e.

$$B(R,T,K,\omega)\Big|_{\alpha\to 0} = 2\pi\delta(\omega - \omega_K) \qquad (4.6.23.)$$

In this limit the phonons behave as non-interacting quasi-phonons with resonant frequencies ω_K (4.6.20.) and group velocities $\bar{v}_K$ (4.4.14.).

We now turn our attentions to the case of non-equilibrium systems driven by the external electric and pressure fields. From (4.3.1.) and (4.3.2.) we see that the electrons are driven directly by an electric field $E_{eff} = -\nabla V_{eff}$ where V_{eff} is given in (4.2.11.) and the phonons are only indirectly affected through the self energy. Consequently the electron spectral function (4.6.17.) will no longer be valid because of the additional energy supplied by the field and we must instead solve a non-equilibrium equation for the spectral function. Generally this is impossible, however under the local-homogeneity-

approximation we may relate the field-dependent spectral function to the equilibrium field independent spectral function as follows.

Because the spectral function is defined as $a(R,T,P,\omega) = g^{>}(R,T,P,\omega) + g^{<}(R,T,P,\omega)$, the equation of motion of the spectral function may be obtained from the corresponding equations of the time ordered Greens functions. We have seen that these equations involve non-local differential driving terms which reduce to local, classical-like expressions under the local-homogeneity approximation in which case from (4.3.24.) and (4.3.25.) the equations may be expressed as

$$[\partial_T + \frac{P}{m}\cdot\partial_R - \partial_R V(R,T)\partial_P - \partial_T V(R,T)\partial_\omega]g^{<}(R,T,P,\omega) = -CI - \mu \quad (4.6.24.)$$

$$[\partial_T + \frac{P}{m}\cdot\partial_R - \partial_R V(R,T)\partial_P - \partial_T V(R,T)\partial_\omega]g^{>}(R,T,P,\omega) = CI + \mu \quad (4.6.25.)$$

with the collision integral given in (4.3.23.) and μ is a function that integrates over (ω) to zero. Consequently adding these two equations together gives us an equation for the electron spectral function valid under the local-homogeneity approximation

$$[\partial_T + \frac{P}{m}\cdot\partial_R + eE(R,T)\cdot\partial_P - \partial_T V(R,T)\partial_\omega]a(R,T,P,\omega) = 0 \quad (4.6.26.)$$

This may be functionally solved by introducing the path variable (τ) which is related to (R,T,P,ω) through

$$\frac{dT}{d\tau} = 1;\ \frac{dR}{d\tau} = \frac{P}{m};\ \frac{dP}{d\tau} = eE;\ \frac{d\omega}{d\tau} = \frac{-\partial V}{\partial T} \quad (4.6.27.)$$

Since (R,T,P,ω) denotes a path in phase-space, the parameter (τ) denotes how far along this path the system has evolved by determining the co-ordinates (R,T,P,ω) as functions of τ.

Explicitly from (4.6.27.) we have

$$\left.\begin{aligned} T &= \tau \\ R(\tau) &= R(0) + \int_0^\tau dt' P(t')/m \\ P(\tau) &= P(0) + \int_0^\tau dt' eE(t') \\ \omega(\tau) &= \omega(0) + V(0) - V(\tau) \end{aligned}\right\} \qquad (4.6.28.)$$

where we have chosen the path variable (τ) to mark time from T = 0 when the fields were suddenly applied.

Thus, in terms of this path variable, the spectral function equation of motion becomes

$$\frac{da(\tau)}{d\tau} = 0$$

or $a(\tau)$ = constant which we take to be evaluated at $\tau = 0$ when our system is assumed to be in equilibrium and in which case the equilibrium spectral function is given by (4.6.17.).

Therefore the field-dependent spectral function is expressible in the form

$$a(\tau) = a(0) = \frac{\Gamma(R(0),P(0),\omega(0))}{[\omega - \bar{\varepsilon}(R(0),P(0),\omega(0))]^2 + [\frac{\Gamma(R(0),P(0),\omega(0))}{2}]^2} \qquad (4.6.29.)$$

where R(0), P(0), $\omega(0)$ are given explicitly as a function of τ and the driving field through (4.6.28.). Thus the value of the non-equilibrium spectral function at a time T after the application of external fields depends on the total previous phase-space trajectory of the system as the above causal integrals show.

The explicit appearance of the effective field in this expression means of course that the collision integrals will be explicitly field dependent, something first considered by Levinson[57] and dubbed the intra-collisional-field-effect by Barker[8]. Before we consider the consequences of this intra-collisional field effect in the collision integrals we must first obtain

expressions for the electron and phonon self energies under the local-homogeneity approximation.

§4.7. The electron and phonon self energies

So far the evolution of the transport theory has unfolded without reference to the precise details of the collision processes, the dynamics of which have been contained within the general expressions of the electron and phonon self-energies defined in terms of the two-electron and mixed electron-phonon Greens function (see (4.2.4.) and (4.2.5.)).

It has long been the burden of many body theorists to try and approximate these higher order Greens functions in terms of single particle quantities as accurately as possible under given circumstances, and yet there are still only basically three methods of approximation. The first may be labelled as inspired physical guesswork, the second is the equation-of-motion technique discussed in §2.3. which leads to a truncation scheme based on asymptotic considerations[79] and the third is a functional derivative technique used in this section.

Although this latter approach may be considered to be the more consistent of the three methods, its' usefulness is probably restricted to high density systems (as we will discuss later) and for low density systems it would still appear that inspired physical guesswork gives the more reliable answers. The difficulty with the functional derivative technique is that it is non-perturbative in nature (a priori we do not know a small parameter in which we may take a polynomial expansion since the fields are large in magnitude and the interactions large in extent) and so it is a problem to determine the precise region of validity of any approximation made, using this method. Consequently we will first obtain an approximation and then discuss its' physical relevance.

We will now see the full strength of working with imaginary time Greens functions in the interaction representation since they readily allow

themselves to be exploited by the functional derivative technique.

If we take first of all the electron self energy in the form introduced in (4.3.3.) i.e.

$$\sum(11') = -i \int d2d3\phi(1 - 2)G(13) \frac{\delta G^{-1}(31')}{\delta V(2)} - i \int d2d3v(1 - 2)G(13) \frac{\delta G^{-1}(31')}{\delta J(2)} \qquad (4.7.1.)$$

where the inverse Greens function defined in (4.3.5.) may be determined from (4.3.1.) in the form

$$G^{-1}(11') = [i\partial_{t_1} + \Delta_1 - V_{eff}(1)]\delta(1 - 1') - \sum(11') \qquad (4.7.2.)$$

We recognise in (4.7.2.) that the inverse Greens function depends on the externally applied fields V(2), J(2) only in so far as it responds to the effective potential $V_{eff}(2)$ (4.2.11.). Therefore it is convenient to use the chain rule to express the functional derivatives of the inverse Greens function in terms of the <u>effective</u> potential so that the self energy becomes

$$\sum(11') = -i \int d2d3d4\phi(1 - 2)G(13) \frac{\delta V_{eff}(4)}{\delta V(2)} \frac{\delta G^{-1}(31')}{\delta V_{eff}(4)} - i \int d2d3d4v(1 - 2)G(13) \frac{\delta V_{eff}(4)}{\delta J(2)} \frac{\delta G^{-1}(31')}{\delta V_{eff}(4)} \qquad (4.7.3.)$$

(4.7.3.) serves to define effective electron-electron and electron-ion interaction potentials respectively by

$$\phi_s(11') = \int d2\phi(1 - 2) \frac{\delta V_{eff}(1')}{\delta V(2)} \qquad (4.7.4.)$$

$$v_s(11') = \int d2v(1 - 2) \frac{\delta V_{eff}(1')}{\delta J(2)} \qquad (4.7.5.)$$

in terms of which the self energy (4.7.3.) is expressible as

$$\sum(11') = -i \int d2d3[\phi_s(1,2) + v_s(1,2)]G(13) \frac{\delta G^{-1}(31')}{\delta V_{eff}(2)} \qquad (4.7.6.)$$

We see from (4.7.6.) that the emphasis of the physical description has swung away from an assembly of interacting electrons and phonons in external fields to one of electrons moving in an effective driving field and interacting only with other electrons through an effective overall electron-electron interaction.

Comparing (4.7.6.) with (4.7.2.) gives a coupled pair of equations, one determining the self energy in terms of the inverse Greens function and the other giving the Greens function in terms of the self energy which need to be solved in a consistent manner. This consistency is supplied by an iterative method generated by the functional derivative since upon substituting (4.7.2.) into (4.7.6.) gives:

$$\sum(11') = i[\phi_s(11') + v_s(11')]G(11')$$

$$- i \int d2d3[\phi_s(1,2) + v_s(1,2)]G(13) \frac{\delta\sum(31')}{\delta V_{eff}(2)} \qquad (4.7.7.)$$

which is a single closed functional derivative equation for the self energy that may be solved iteratively. Since such a functional derivative equation has no known exact method of solution, the approximation we take is to assume that

$$\frac{\delta\sum(11')}{\delta V_{eff}(2)} = 0 \qquad (4.7.8.)$$

so that the self energy is given in terms of the effective interactions as

$$\sum(11') = i[\phi_s(11') + v_s(11')]G(11') \qquad (4.7.9.)$$

This level of approximation has been used by various authors in the past concerned with the electron plasma who found that it led to a generalised Born description of the collision processes[26][51]. To my knowledge no-one has yet managed to include higher order correlations consistently than the level determined by (4.7.8.) and still obtain a meaningful transport equation. However, it is possible to obtain an approximation for $\delta\sum/\delta V_{eff} \neq 0$ under the

local-homogeneity approximation as is demonstrated for the first time in Appendix V. This higher level of approximation is not considered explicitly in this section because we consider the level determined by (4.7.8.) to be sufficient for our purposes by the following justification.

Even though the functional derivative technique is non-perturbative, it is still possible to obtain physical estimates for the range of validity of the approximation (4.7.8.) as follows. We have seen using the local-homogeneity-approximation that the real and imaginary parts of the self energy contribute to the dynamics in different ways. If the imaginary part is zero then the electron has a singular spectral relation; there is no collision broadening and the particle behaves as free but with a modified energy. Therefore we may consider the effective driving field as including the real part of the self energy and the randomising effect usually associated with collisions which forces a spread in the energy distribution is due to the imaginary part.

We may loosely think of the electron motion as divided into two regions: a finite randomising collision event and free motion between collisions in an effective driving field. If we change the field we will vary the amount of energy an electron picks up from the field between and during collisions. Therefore if the collisionless "free-particle" part of the electron Greens function is denoted by G_0, the assumption leading to (4.7.9.) is just

$$\frac{\delta \Sigma}{\delta V_{eff}} << \frac{\delta G_0}{\delta V_{eff}}$$

so that the energy picked up from the field between collisions is much greater than that picked up within a collision.

This may be converted into an inequality for the electron density if we assume the effective field is constant, since then the energy picked up is just proportional to the distances involved. For an electron density of n cm^{-3}, the mean distance between scattering centres is $1/n^{1/3}$. If the collision cross-section is estimated by assuming that the interaction is

screened out, outside a distance of the order of the Debye screening length[72]

$$\lambda_D = \sqrt{\frac{\epsilon k_B T}{ne^2}}$$

then we have that the distance between collisions is just

$$d_{free} = 1/n^{1/3} - 2\lambda_D$$

Therefore assuming that the energy picked up between collisions is much greater than that picked up within an event means that the mean free distance is greater than the length occupied by a collision process so that

$$1/n^{1/3} > 4\lambda_D \quad \text{or} \quad n > 16 \left[\frac{\epsilon k_B T}{e^2}\right]^3 \qquad (4.7.10.)$$

Typically for $\epsilon = 10\ \epsilon_0$ at T = 300 K, this inequality requires a density in excess of 10^{15} cm^{-3}. This is quite large and perhaps is a feature of overestimating the collisional region by the Debye screening length. (Note that the argument would remain valid had we used a Thomas-Fermi screening length[39][60] since it still varies as the inverse square root of the density.)

However, even though (4.7.10.) probably overestimates the critical density, it is still well below the typical doping levels of 10^{16} - 10^{18} cm^{-3} required in the medium-small-device and so we anticipate that the approximation leading to the self energy expression (4.7.9.) is a good one to make for our situation.

This is why it was mentioned at the start of this section that the functional derivative technique is limited to high density systems but it is interesting to speculate what happens as the density decreases. In this case the screening length ($\propto 1/\sqrt{n}$ increases faster than the mean separation between electrons ($\propto 1/n^{1/3}$) until a critical density is reached where the collision radii begin to overlap: the carrier is swept on into subsequent collisions before its' original one had been completed and long range

correlations will build up in the system due to these overlapping interactions. The effects of such long range correlations cannot be described by the approximation (4.7.9.) although various people have postulated the formation of a Wigner lattice as a consequence of these low density long range interactions.

Going back to our approximation (4.7.9.), it may be Wigner transformed under the local-homogeneity-approximation to give

$$\Sigma^{\gtrless}(R,T,P,\omega) = \int d^3P' \frac{d\omega'}{2\pi} [\phi_S^{\gtrless}(R,T,P',\omega') + v_S^{\gtrless}(R,T,P',\omega')] \times g^{\gtrless}(R,T,\ P - P',\omega - \omega') \qquad (4.7.11.)$$

where the Wigner transform of the effective interactions have yet to be evaluated. Note that these effective interactions are now causal functions in distinction to the bare interactions which were instantaneous. This may be directly seen from the definitions of the effective interactions (4.7.4.) and (4.7.5.) and using the explicit definition of the effective potential (4.2.11.) in which case we have exactly

$$\phi_S(11') - \phi(1 - 1') = \int d2d3\phi(1 - 2)[\phi(1' - 3)\{iG_2(22^+33^+) - iG(22^+)G(33^+)\} \pm v(1' - 3)[\frac{<TSq(3)\psi(2)\psi^\dagger(2^+)>}{<TS>} - Q(3)G(22^+)\}] \qquad (4.7.12.)$$

and

$$v_S(11') = \int d2d3v(1 - 2)[\pm \phi(1' - 3)\{\frac{<TSq(2)\psi(3)\psi^\dagger(3^+)>}{<TS>} - Q(2)G(33^+)\} + v(1' - 3)D(3,2)] \qquad (4.7.13.)$$

It is easily seen from these definitions that the effective interactions are governed by density-density correlation functions which themselves are all causal functions.

In order to obtain approximate expressions for these effective interactions it is thus necessary to insert an approximation for the correlation functions consistent with the approximation that led to the self energy (4.7.9.).

Therefore from (4.7.4.) and inserting the definition of the effective potential (4.2.11.) we find

$$\phi_s(11') - \phi(1 - 1') = \int d2d3\phi(1 - 2)[\pm i\phi(1' - 3) \frac{\delta G(33^+)}{\delta V(2)} + v(1' - 3) \frac{\delta Q(3)}{\delta V(2)}]$$

$$= \pm i \int d2d3\{\phi(1 - 2)\phi(1' - 3) \frac{\delta G(33^+)}{\delta V(2)}$$

$$+ \phi(1' - 3)v(1' - 2) \frac{\delta G(33^+)}{\delta J(2)}\} \qquad (4.7.14.)$$

where we have made use of the functional derivative identity (III.10.). We may now use the chain rule to convert (4.7.14.) into an expression involving the functional derivative with respect to the effective potential to give

$$\phi_s(11') - \phi(1 - 1') = \mp i \int d3d4d5d6G(34^+)G(53^+)\frac{\delta G^{-1}(45^+)}{\delta V_{eff}(6)}$$

$$x \{\phi(1' - 3)\phi_s(1,6) + \phi(1 - 3)v_s(1',6)\} \qquad (4.7.15.)$$

We are now in a position to use the inverse Greens function equation (4.7.2.), functionally differentiate with respect to the effective driving field and neglect the self energy derivative as in (4.7.8.) to give an approximate integral equation for the effective electron interaction

$$\phi_s(11') - \phi(1 - 1') = \pm i \int d2d3\{\phi(1' - 3)\phi_s(1,2) +$$

$$+ \phi(1 - 3)v_s(1',2)\}G(23)G(32^+) \qquad (4.7.16.)$$

This integral form is converted into an algebraic form by Wigner transforming under the local-homogeneity-approximation which yields

$$\phi_s(R,T,P,\omega) - \phi(P) = \phi_s(R,T,P,\omega)\phi(P)L(RTP\omega)$$

$$+ v_s(R,T,P,\omega)\phi(P)L(RTP\omega)$$

or

$$\phi_s(R,T,P,\omega) = \frac{[\phi(P) + \phi(P)L(RTP\omega)v_s(RTP\omega)]}{1 - \phi(P)L(RTP\omega)} \qquad (4.7.17.)$$

where $L(R,T,P,\omega)$ is the Wigner transform of $\pm iG(23)G(32^+)$ given explicitly by

$$L(R,T,P,\omega) = \int \frac{d\omega'}{2\pi} \frac{[L^>(RTP\omega') - L^<(RTP\omega')]}{\omega - \omega'} \qquad (4.7.18.)$$

where $L^{\gtrless}$ is the Wigner transform of $\pm iG^{\gtrless}(23^+)G^{\lessgtr}(32^+)$ i.e.

$$L^{\gtrless}(RTP\omega) = \int d^3P' \frac{d\omega'}{2\pi} G^{\gtrless}(R,T,P+P',\omega+\omega')G^{\lessgtr}(R,T,P',\omega')$$

$$= \int d^3P' \frac{d\omega'}{2\pi} G^{\gtrless}(R,T,P' + \frac{P}{2},\omega' + \frac{\omega}{2})G^{\lessgtr}(R,T,P' - \frac{P}{2},\omega' - \frac{\omega}{2}) \qquad (4.7.19.)$$

We now wish to obtain the effective electron-phonon interaction which is obtained in a similar fashion. Using the definition (4.7.5.) and (4.2.11.) we have exactly

$$v_s(11') = \int d2d3v(1-2)[\pm i\phi(1'-3)\frac{\delta G(33^+)}{\delta J(2)} +$$

$$+ v(1'-3)\frac{\delta Q(3)}{\delta J(2)}] \qquad (4.7.20.)$$

Using the relationship (III.10.) and converting to effective functional derivatives of the inverse Greens function reduces (4.7.20) to the form:

$$v_s(11') = \int d2d3v(1-2)D(32)$$

$$\mp i \int d3d4d5d6v_s(1,6)\phi(1'-3)G(34)G(53^+)\frac{\delta G^{-1}(45)}{\delta V_{eff}(6)} \qquad (4.7.21.)$$

To the same level of approximation as in the electron case, (4.7.21.) approximates to an integral equation for v_s, specifically

$$v_s(11') = \int d2d3v(1-2)v(1'-3)D(3,2) \pm$$

$$\pm i \int d2d3v_s(12)\phi(1'-3)G(23^+)G(32^+) \qquad (4.7.22.)$$

Again this may be Wigner transformed under the local homogeneity approximation to give the algebraic expression

$$v_s(RTP\omega) = \frac{|v(P)|^2 D(RTP\omega)}{1 - \phi(P)L(RTP\omega)} \qquad (4.7.23.)$$

where $L(RTP\omega)$ is the same quantity defined in (4.7.18.). We may now combine (4.7.17.) with (4.7.23.) to obtain an expression for the combined effective interaction potential $\phi_s + v_s$ that appears in the self energy expression (4.7.11.). Explicitly

$$[\phi_s(RTP\omega) + v_s(RTP\omega)] = \frac{\phi(P)}{1 - \phi(P)L(RTP\omega)} +$$

$$+ \left|\frac{v(P)}{1 - \phi(P)L(RTP\omega)}\right|^2 D(RTP\omega) \qquad (4.7.24.)$$

What we are really concerned with though are the time ordered components of the causal function $C = \phi_s + v_s$ in (4.7.24.). However from the Lehmann spectral representations (see (II.27.)) we know that $C^>(P\omega) + C^<(P\omega) \equiv 2\mathrm{Im}C(P,\omega - i\delta)$ which from (4.7.24.) is just

$$\left|\frac{\phi(P)}{\epsilon(RTP\omega - i\delta)}\right|^2 2\mathrm{Im}L(\omega - i\delta) + \left|\frac{v(P)}{\epsilon(RTP\omega - i\delta)}\right|^2 2\mathrm{Im}D(\omega - i\delta)$$

$$= \left|\frac{\phi(P)}{\epsilon(RTP\omega - i\delta)}\right|^2 [L^>(RTP\omega) + L^<(RTP\omega)]$$

$$+ \left|\frac{v(P)}{\epsilon(RTP\omega - i\delta)}\right|^2 [D^>(RTP\omega) + D^<(RTP\omega)] \qquad (4.7.25.)$$

If we also make use of the time reversal symmetry which implies that $L^>(P\omega) = L^<(-P-\omega)$; $D^>(P\omega) = D^<(-P,-\omega)$ then (4.7.25.) leads to expressions for the time ordered effective interactions

$$C^{\gtrless} = [\phi_S^{\gtrless}(RTP\omega) + v_S^{\gtrless}(RTP\omega)] = \left|\frac{\phi(P)}{\epsilon(RTP\omega - i\delta)}\right|^2 L^{\gtrless}(RTP\omega) +$$

$$+ \left|\frac{v(P)}{\epsilon(RTP\omega - i\delta)}\right|^2 D^{\gtrless}(RTP\omega) \qquad (4.7.26.)$$

We see from the above expressions that the effect of the interactions has been to renormalise the bare interaction potentials by dividing by a function

$$\epsilon(RTP\omega) = 1 - \phi(P)L(RTP\omega) \qquad (4.7.27.)$$

which is known as the screening function. Since the next chapter is devoted to considerations of this screening function particularly with regard to its' dependence on the effective driving field, we only comment here that (4.7.27.) depends non-linearly on the non-equilibrium distribution function itself as can be seen from (4.7.19.), and therefore must be evaluated self consistently within the transport equations.

We have thus managed to obtain an approximate form for the electron self energy by using a combination of neglecting certain correlations and Wigner transforming under the local homogeneity approximation. Using this procedure we will now briefly obtain the equivalent approximation to the phonon self energy as much of the analysis is identical. From definition (4.3.4.) we know

$$\pi(11') = i \int d2V^{\dagger}(1) \frac{\delta G(11^+)}{\delta J(2)} D^{-1}(2,1')$$

$$= -i \int d2d3d4V^{\dagger}(1)G(13)G(41^+) \frac{\delta G^{-1}(34^+)}{\delta J(2)} D^{-1}(21')$$

$$= -i \int d2d3d4d5V^{\dagger}(1)G(13)G(41^+) \frac{\delta V_{eff}(5)}{\delta J(2)} D^{-1}(21') \frac{\delta G^{-1}(34^+)}{\delta V_{eff}(5)}$$

$$(4.7.28.)$$

Making use of the first iterative approximation (4.7.8.), (4.7.28.) reduces to

$$\pi(11') = i \int d2d5V^{\dagger}(1)G(15^{+})G(51^{+})\frac{\delta V_{eff}(5)}{\delta J(2)} D^{-1}(21')$$

$$= i \int d2d5V^{\dagger}(1)G(15^{+})G(51^{+})D^{-1}(21') \; x$$

$$x \{\pm i\phi(5) \frac{\delta G(55^{+})}{\delta J(2)} + v(5) \frac{\delta Q(5)}{\delta J(2)}\} \qquad (4.7.29.)$$

where we have substituted in for V_{eff}. Using identity (III.9), this equation further becomes

$$\pi(11') = iV^{*}(1)G(11')G(1',1^{+})V(1')$$

$$+ i \int d2d5V^{*}(1) \frac{\delta G(55^{+})}{\delta J(2)} D^{-1}(21')(\pm i)\phi(5)G(15)G(51^{+})$$

which can be Wigner transformed using the local homogeneity approximation and the definition of $\pi(11')$ to give

$$\pi(RTK\omega) = -|V|^{2}L(RTK\omega) + \pi(RTK\omega)\phi(K)L(RTK\omega)$$

$$= \frac{-|V(K)|^{2}L(RTK\omega)}{1 - \phi(K)L(RTK\omega)} \qquad (4.7.30.)$$

Again we are only interested in the time ordered variants of (4.7.30.) which as before depends on the imaginary part of π. The analysis gives

$$\pi^{\gtrless}(RTK\omega) = -\left|\frac{V(K)}{\epsilon(RTK\omega - i\delta)}\right|^{2} L^{\gtrless}(RTK\omega) \qquad (4.7.31.)$$

where again the effect of interactions is to renormalise the bare interaction potential by dividing by the same screening function (4.7.27.).

Before we construct the final transport equations using these approximate self energy expressions, we now consider, as an illustrative exercise, a diagram analysis of the first-iterative-approximation used in this section.

§4.8. A diagram analysis of the first-iterative, or nesting, approximation

In the preceding section a level of approximation to the correlations was introduced (4.7.8.) which will now be considered by the use of diagrams. We will work with double time Greens functions directly since then a vertex in a diagram will refer to the co-ordinate pair (r,t). Throughout this section

we attempt to adhere to the notation of Mattuck[66] although the diagrams are generally self explanatory.

Thus for simplicity we consider first the case of electron-electron interactions only, determined by the equation

$$[i\partial_{t_1} + \Delta_1 - V(1)]G(11') \mp i\int d2\phi(1-2)G_2(11'22^+) = \delta(1-1') \qquad (4.8.1.)$$

which has the structural form of

$$G_0^{-1}(11')G(11') - \int d\bar{1}\sum{}'(1\bar{1})G(\bar{1}1') = \delta(1-1') \qquad (4.8.2.)$$

where $G_0^{-1}(11') \equiv [i\partial_{t_1} + \Delta_1 - V(1)]\delta(1-1')$ is the inverse Greens function propagator for a free electron (no interactions) moving under the influence of an external potential. We denote this free Greens function propagator by a directed dash-dot line where the starting point corresponds to (r_1,t_1) and ends at (r_1',t_1').

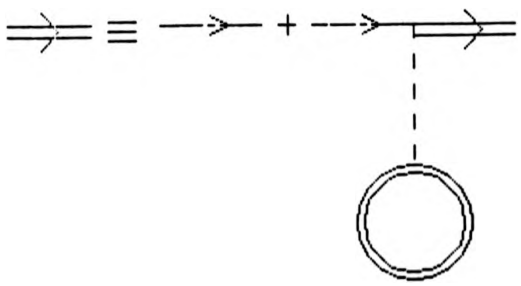
Under the Hartree approximation where the two-electron Greens function is assumed to be

$$G_2(11'22') = G(11')G(22') \qquad (4.8.3.)$$

then (4.8.1.) is manipulated into an iterative expression for the Hartree approximation to the one electron Greens function G_H as

$$G_H(11') \equiv G_0(11') + i\int d2d3\phi(3-2)G_0(13)G_H(31')G_H(22^+) \qquad (4.8.4.(i))$$

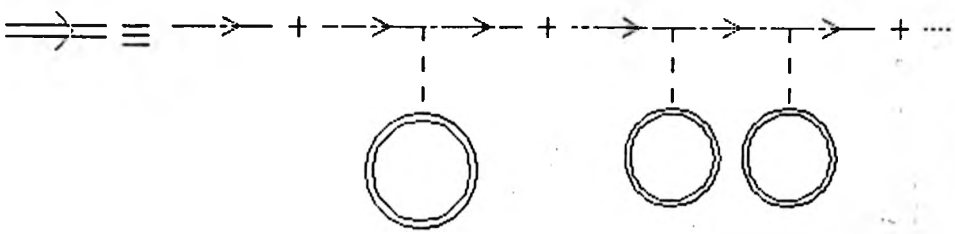
represented in diagramatic form thus:



(4.8.4.(ii))

where double lines throughout this section refer to renormalised quantities.

This self-consistent expansion (4.8.4.) is usually represented by the infinite series



which is known as the sum of bubble diagrams[65]. These 'bubbles' are the polarisation parts of a particle interacting with a medium which acts back on the particle producing an effective potential. The particle-medium interaction in this case is pure Coulombic (represented by the single dashed line in the above diagrams) and as such, this level of approximation does not produce any lifetime broadening.

Therefore, the Hartree approximation corresponds to a free electron moving under the influence of an effective potential which includes to some extent the polarisation of the medium through (4.8.3.). Consequently we denote this free electron propagator by a single unbroken line corresponding to the infinite expansion (4.8.4.(ii)).

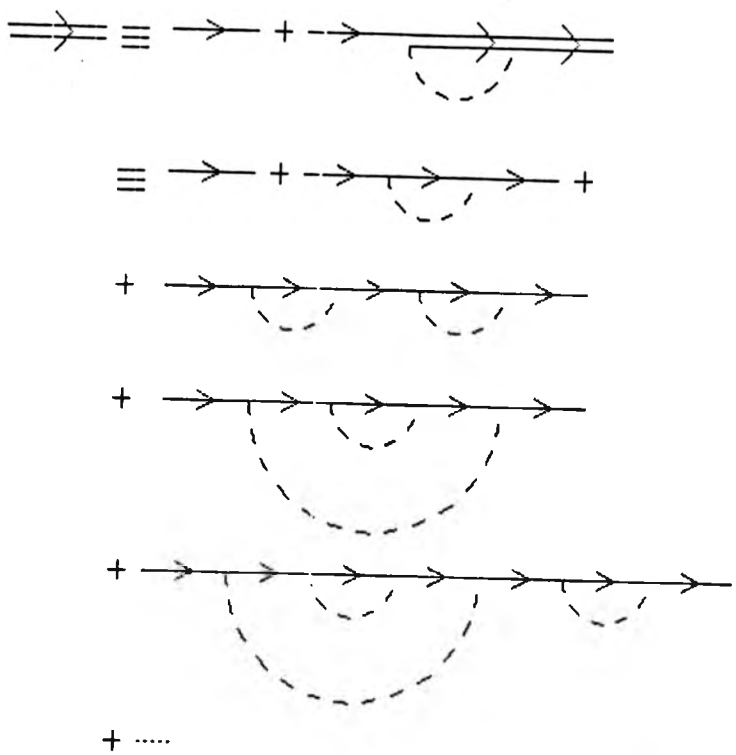
This simplifies all subsequent algebra and diagrams, since for example in the next level of approximation given by the Hartree-Fock contribution where the two-electron Greens function includes exchange terms as:

$$G_2(11'22') = G(11')G(22') - G(12')G(21') \qquad (4.8.5.)$$

the resulting approximation to the one-electron Greens function is representible as

$$G_{HF}(11') = G_1(11') - i \int d2d3\phi(3 - 2)G_1(13)G_{HF}(32^+)G_{HF}(21') \qquad (4.8.6.(i))$$

which, in terms of diagrams takes the form



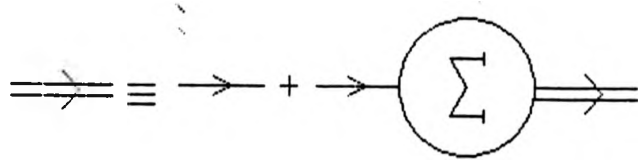
(4.8.6.(ii))

sometimes refered to as an 'open-oyster' expansion[66].

We can now use the effective free propagator to analyse the self energy since from (4.3.1.) we have

$$G(11') = G_1(11') + \int d\bar{1}d2G_1(12)\Sigma(2\bar{1})G(\bar{1}1') \qquad (4.8.7.(i))$$

or

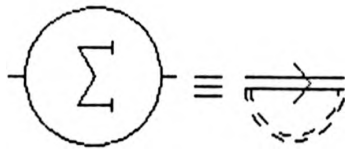


(4.8.7.(ii))

Under the first iterative qpproximation used in this chapter the self-energy is determined by (4.7.9.)

$$\Sigma(11') = i\phi_s(11')G(11') \qquad (4.8.8.(i))$$

or

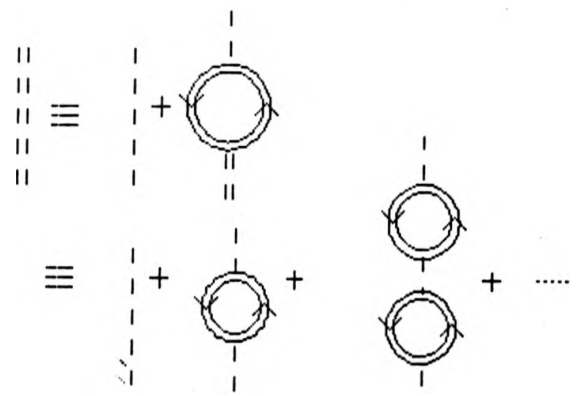


(4.8.8.(ii))

where the effective electron-electron interaction $\phi_s(11')$ is, to the same degree of approximation given by (4.7.16.)

$$\phi_s(11') = \phi(1 - 1') + \int d3d4\phi_s(14)\phi(1' - 3)(-i)G(34)G(43^+) \qquad (4.8.9.(i))$$

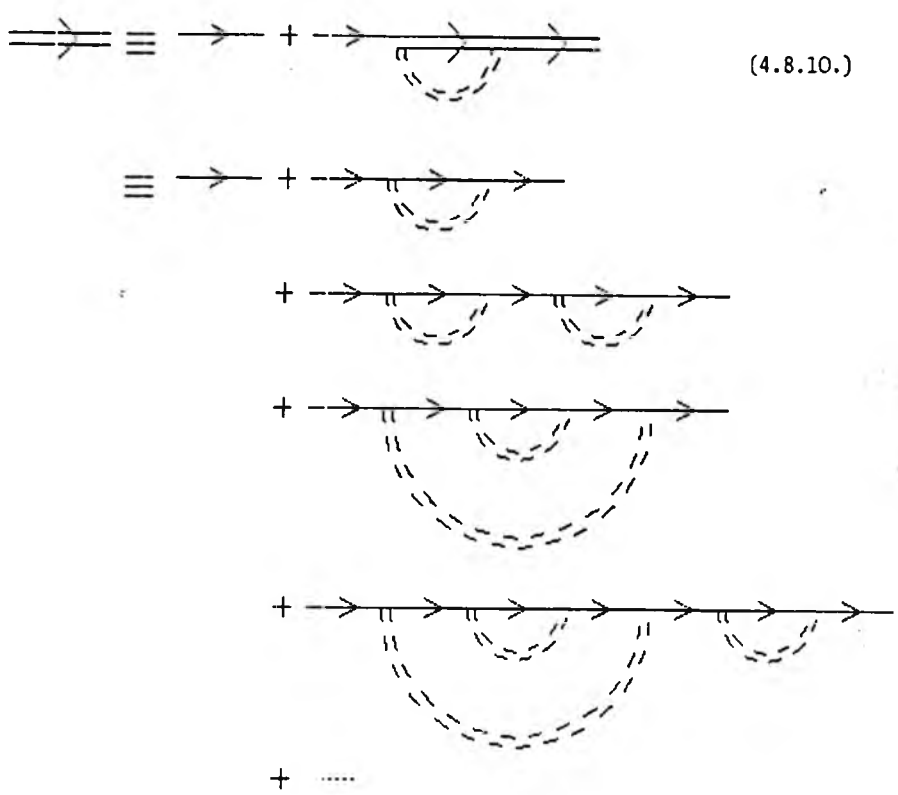
or



(4.8.9.(ii))

We can see by comparing (4.8.9.(ii)) with (4.8.4.(ii)) that the effective interaction potential also results from an infinite sum of bubble diagrams connected by bare propagators thus demonstrating the explicit intervention of the surrounding medium in the dynamics.

Expanding the self-energy (4.8.8.(ii)) in (4.8.7.(ii)) gives the approximate one electron Greens function:



(4.8.10.)

from which (upon comparing with (4.8.6.(ii)) and using (4.8.9.(ii)) it is clear that the first iterative approximation includes the Hartree-Fock level of description as a subset.

It is also interesting to note from (4.8.10.) that this approximation cannot allow propagators to cross each other - they can only nest inside each other which explains the alternative nomenclature: the nesting approximation.

The comparison between (4.8.10.) and (4.8.6.(ii)) demonstrates that this nesting approximation is similar to a Hartree-Fock approximation except that the electron-medium interaction proceeds not by the bare Coulomb interaction but by a retarded effective interaction (4.8.9.). This may also be seen in the symbolic decomposition of the two-electron Greens function as follows.

We have seen that, in terms of functional derivatives we have exactly (III.6.)

$$G_2(11'22^+) = G(11')G(22^+) - \frac{\delta G(11')}{\delta V(2)} \qquad (4.8.11.)$$

where, under the nesting approximation the functional derivative is expressed in terms of single electron propagators as

$$\frac{\delta G(11')}{\delta V(2)} = G(12^+)G(21') - i \int d3d4\phi(3 - 4)G(13)G(31') \frac{\delta G(44^+)}{\delta V(2)} \qquad (4.8.12.)$$

If we Wigner transform (4.8.12.) under the local-homogeneity-approximation, the algebraic equivalent of the functional derivative becomes

$$\frac{\delta G}{\delta V} = \frac{\hat{GG}}{1 - \phi L} \qquad (4.8.13.)$$

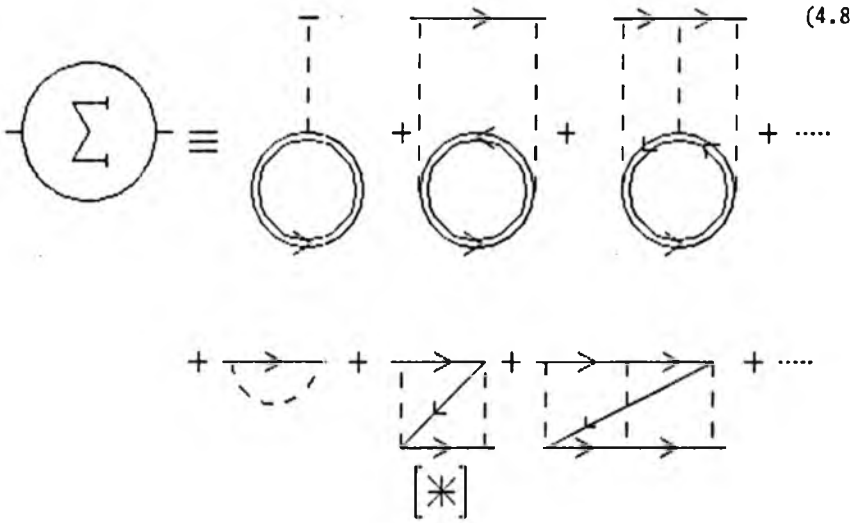
where $\hat{GG}$ refers to the exchange Greens functions and L was introduced in the previous section (4.7.18.).

Using this result in (4.8.11.) allows us to interpret the nesting approximation as splitting the two-electron Greens function into the product of two one-electron Greens functions (the Hartree approximation) plus an exchange contribution which is reduced (screened) due to the polarisation of the medium.

This is a much more satisfying state of affairs since we no longer overestimate the contribution of the exchange effects as in the naive Hartree-Fock approximation, and furthermore the self energy will now have an imaginary component due to the frequency dependent, retarded screening function leading to finite lifetime quasi particles.

Unfortunately (as discussed in the previous section) the nesting approximation is not applicable to low density systems as is possible to demonstrate using diagram methods.

It is already understood[60][66] that the dominant contribution to the self-energy in the low density system comes from the "ladder approximation" as defined by the infinite sum of diagrams:

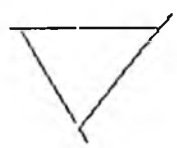


(4.8.14.)

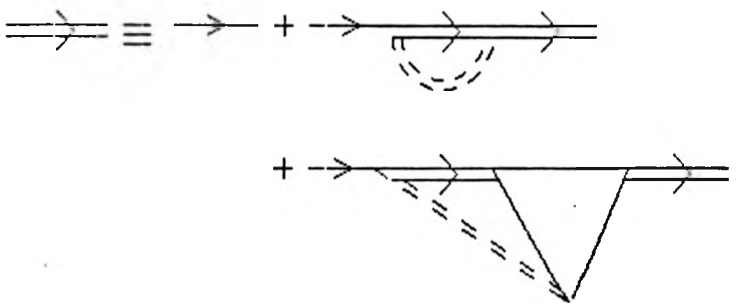
We now show that these diagrams can only be generated by going to a higher level of approximation than determined by the nesting approximation (4.7.8.).

From (4.8.7.(i)) and the appropriate self-energy definition (4.7.6.) we have

$$G(11') = G_1(11') + i\int d\bar{1}d2G_1(12)\phi_s(2\bar{1})G(2\bar{1})G(\bar{1}1') + i\int d\bar{1}d2d3d4G_1(12)\phi_s(23)G(24)G(\bar{1}1')\frac{\delta\Sigma(4\bar{1})}{\delta V(3)} \quad (4.8.15.(i))$$

This is an exact expression for the one-electron Greens function involving a three-point correlation function $\delta\Sigma(4\bar{1})/\delta V(3)$ for which we introduce the new diagram  so that (4.8.15.) may be cauched in

diagrammatic terms as:-



(4.8.15.(ii))

It is clear from this expansion that the three-point correlation function corresponds in general to a dressed vertex (note that this is the logical extension of a quasi-particle theory developed in terms of renormalised propagators, renormalised interactions and subsequently renormalised vertices). Note that the nesting approximation only gives the first two terms in the expansion (4.8.15.(ii)) and assumes the vertex is unrenormalised.

The ladder approximation is involved within this renormalised vertex since an expansion of the three-point correlation gives

$$\frac{\delta\Gamma(4\bar{1})}{\delta V(3)} = -i \int d6d7\phi_s(46) \frac{\delta}{\delta V(3)} [G(47) \frac{\delta G^{-1}(7\bar{1})}{\delta V(6)}]$$

$$= i\phi_s(4\bar{1}) \frac{\delta G(4\bar{1})}{\delta V(3)}$$

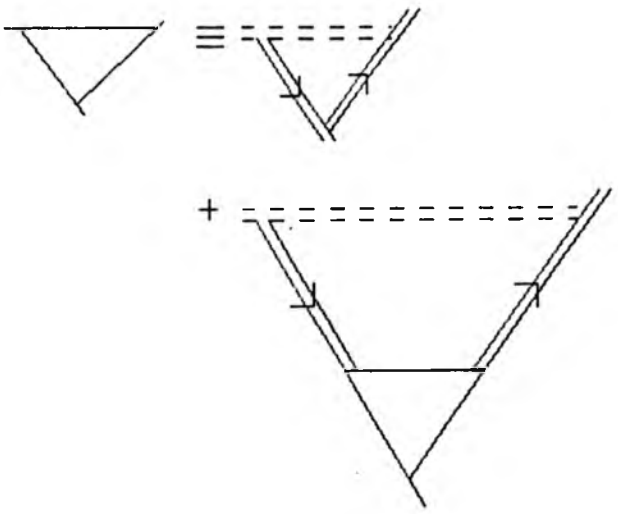
$$+ i \int d6d7\phi_s(46) \frac{\delta}{\delta V(3)} [G(47) \frac{\delta\Gamma(7\bar{1})}{\delta V(6)}]$$

which upon neglecting terms governed by $\delta^2\Gamma/\delta V^2$ gives

$$\frac{\delta\Gamma(4\bar{1})}{\delta V(3)} = i\phi_s(4\bar{1})G(43)G(3\bar{1}) +$$

$$+ i\phi_s(4\bar{1}) \int d6d7G(46)G(7\bar{1}) \frac{\delta\Gamma(67)}{\delta V(3)} \qquad (4.8.16.(i))$$

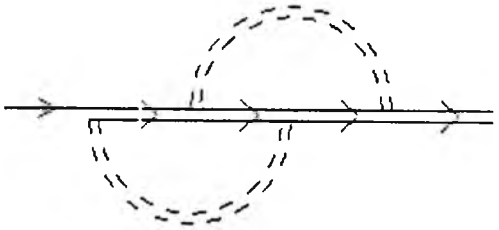
with a diagrammatic representation:



(4.8.16.(ii))

If we just use the first diagram of this approximation it gives a vertex correction to the one electron propagator of

(4.8.17.)



However it is clear that the lowest order expansion of (4.8.17.) is precisely the diagram in the ladder approximation (4.8.14.) marked with an asterisk. Consequently we recognise that the ladder approximation is contained within the vertex corrections which in turn are governed by a higher order of approximation than that given by the nesting approximation. Therefore we may take this diagrammatic argument as supplementing the physical justification given in §4.7. that the nesting approximation is restricted to high density systems.

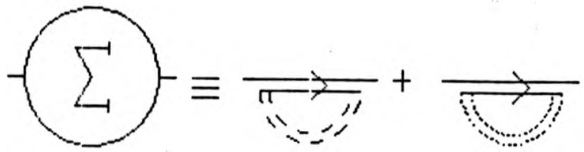
The diagram expansion is easily extended to involve electron-phonon interactions with the bare (dressed) electron-phonon interaction denoted by

single (double) dots and with the phonon correlation function D(11') represented by a long rectangle.

Thus the nesting approximation for the electron self-energy is given in (4.7.9.) as

$$\Sigma(11') = i[\phi_s(11') + v_s(11')]G(11') \qquad (4.8.18.(i))$$

or

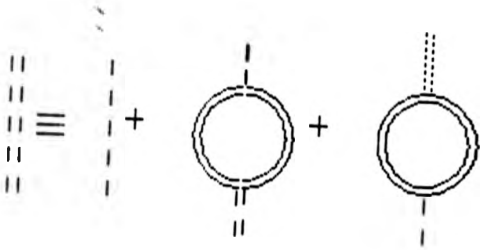


(4.8.18.(ii))

where the effective electron-electron and electron-phonon interactions are similarly represented under the nesting approximation from (4.7.16.) and (4.7.22.) as

$$\phi_s(11') = \phi(1 - 1') - i \int d3d4[\phi_s(14)\phi(1' - 3) + \phi(1 - 3)v_s(1'4)]G(34)G(43^+) \qquad (4.8.19.(i))$$

i.e.

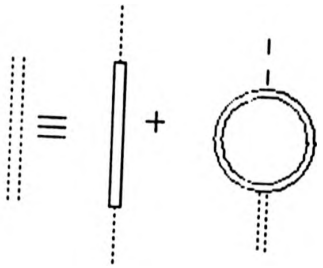


(4.8.19.(ii))

and

$$v_s(11') = \int d3d4[v(1 - 3)v^*(1' - 4)D(34) - i\phi(1' - 3)v_s(14)G(34)g(43^+)] \qquad (4.8.20.(i))$$

i.e.



(4.8.20.(ii))

This set of diagrams (4.8.18)-(4.8.20.) characterises the nesting approximation to the dynamics of collisions in our coupled electron-electron-phonon system.

Of course it is possible as (4.8.18.) shows to eliminate the need for separate electron-electron and electron-phonon interactions in favour of an effective, retarded electron-electron interaction as for example prefered in theories of superconductivity[60][66]. However it is important to recognise that the separate interactions constituting the effective potential are themselves already retarded through the many body effects of electron-electron interactions.

The diagrams for the effective interactions are coupled iterative representations of infinite sums of various classes of diagrams which in general are impossible to decouple. It is the use of the local-homogeneity-approximation combined with the nesting approximation that allows a decomposition of the effective interaction into the sum of screened electron-electron and electron-phonon interactions as performed in §4.7.

§4.9. The electron and phonon Wigner distribution transport equations

We are now in a position to synthesise the various components of this chapter into a coupled pair of transport equations for the one-electron

and one-phonon Wigner distributions appropriate to non-equilibrium high field conditions in the medium-small-device.

The model Hamiltonian (4.1.1.) manipulated using Greens functions techniques and approximated by the local-homogeneity assumption (§4.5.) led to equations of motion of the form

$$[\partial_T + \frac{P}{m}\cdot\partial_R + F(R,T)\cdot\partial_P]f(R,P,T) = \left.\frac{-\partial f}{\partial T}\right|_{coll} \qquad (4.9.1.)$$

$$[\partial_T + \bar{v}_K\cdot\partial_R]n(R,K,T) = \left.\frac{-\partial n}{\partial T}\right|_{coll} \qquad (4.9.2.)$$

where the collision integrals are obtained by inserting the self energy expressions (4.7.11.) and (4.7.31.) calculated under the nesting approximation (§4.8.) into (4.5.13.) and (4.5.14.) which gives explicitly:

$$\begin{aligned}\left.\frac{\partial f}{\partial T}\right|_{coll} = &\int \frac{d\Omega'}{2\pi}\frac{d\Omega''}{2\pi}\int_0^T d\tau a(R,P,\Omega'',\tau)\{2e^{2i(\Omega'-\Omega'')(T-\tau)} + c.c.\}\\ &\times \int d^3p' \frac{d\omega'}{2\pi} a(R,\tau,P-P',\Omega'-\omega')\\ &\times \{[\phi_s^>(R,P',\tau,\omega') + v_s^>(R,P',\tau,\omega')]f(R,P,\tau)[1-f(R,P-P',\tau)]\\ &- [\phi_s^<(R,P',\tau,\omega') + v_s^<(R,P',\tau,\omega')]f(R,P-P',\tau)[1-f(R,P',\tau)]\}\end{aligned} \qquad (4.9.3.)$$

and

$$\begin{aligned}\left.\frac{\partial n}{\partial T}\right|_{coll} = &\int \frac{d\Omega'}{2\pi}\frac{d\Omega''}{2\pi}\int_0^T d\tau \frac{b(R,K,\Omega'',\tau)}{2\omega_K}\{2e^{2i(\Omega'-\Omega'')(T-\tau)} + c.c.\}\\ &\times \left|\frac{v(K)}{\epsilon(R,K,\tau,\Omega'-i\delta)}\right|^2 L^>(R,K,\tau,\Omega'')n(R,K,\tau)\\ &- L^<(R,K,\tau,\Omega'')[1+n(R,K,\tau)]\}\end{aligned} \qquad (4.9.4.)$$

If we now use the approximations obtained in (4.7.24.) for the two branches of the effective electron interaction, $\phi_s + v_s$, we find the electron collision integral splits into electron-electron and electron-phonon components,

i.e. $$\left.\frac{\partial f}{\partial T}\right|_{coll} \equiv \left.\frac{\partial f}{\partial T}\right|_{e\text{-}e} + \left.\frac{\partial f}{\partial T}\right|_{e\text{-}ph} \qquad (4.9.5.)$$

where

$$\left.\frac{\partial f}{\partial T}\right|_{e\text{-}e} = \int \frac{d\Omega'}{2\pi}\frac{d\Omega''}{2\pi}\frac{d\omega'}{2\pi}\frac{d\omega''}{2\pi} d^3p' d^3p'' \int_0^T d\tau\{2e^{2i(\Omega'-\Omega'')(T-\tau)} + c.c.\}$$

$$x\ a(R,P,\Omega'',\tau)a(R,P-P',\Omega'-\omega',\tau)a(R,P'',\omega'',\tau)a(R,P'+P'',\omega'+\omega'',\tau)$$

$$x\left|\frac{\phi(P')}{\epsilon(R,\tau,P',\omega'-i\delta)}\right|^2$$

$$x\{f(R,P,\tau)[1-f(R,P-P',\tau)]f(R,P'',\tau)[1-f(R,P'+P'',\tau)]$$

$$-[1-f(R,P,\tau)]f(R,P-P',\tau)[1-f(R,P'',\tau)]f(R,P'+P'',\tau)\} \qquad (4.9.6.)$$

and

$$\left.\frac{\partial f}{\partial T}\right|_{e\text{-}ph} = \int \frac{d\Omega'}{2\pi}\frac{d\Omega''}{2\pi}\frac{d\omega'}{2\pi} d^3p' \int_0^T d\tau\{2e^{2i(\Omega'-\Omega'')(T-\tau)} + c.c.\}$$

$$x\left|\frac{v(P')}{\epsilon(R,P',\tau,\omega'-i\delta)}\right|^2 a(R,P,\tau,\Omega'')a(R,P-P',\tau,\Omega'-\omega')$$

$$x(f(R,P,\tau)[1-f(R,P-P',\tau)]\{\frac{b(R,\tau,P',\omega')}{2\omega_K}[1+n(R,\tau,P')] +$$

$$+\frac{b(R,\tau,-P',-\omega')}{2\omega_K}n(R,\tau,-P')\}$$

$$-[1-f(R,P,\tau)]f(R,P-P',\tau)\{\frac{b(R,\tau,P',\omega')}{2\omega_K}n(R,\tau,P') +$$

$$+\frac{b(R,\tau,-P',-\omega')}{2\omega_K}[1+n(R,\tau,-P')]\}) \qquad (4.9.7.)$$

Similarly we find the phonon collision integral expressible as

$$\left.\frac{\partial n}{\partial T}\right|_{e\text{-}ph} = \int \frac{d\Omega'}{2\pi}\frac{d\Omega''}{2\pi}\frac{d\Omega'}{2\pi} d^3K' \int_0^T d\tau\{2e^{2i(\Omega'-\Omega'')(T-\tau)} + c.c.\}$$

$$x\frac{b(R,K,\tau,\Omega'')}{2\omega_K}a(R,K+K',\Omega''+\omega',\tau)a(R,K',\omega',\tau)$$

$$x\left|\frac{v(K)}{\epsilon(R,K,\tau,\Omega''-i\delta)}\right|^2\{f(R,K',\tau)[1-f(R,K+K',\tau)]n(R,K,\tau)$$

$$-[1-f(R,K',\tau)]f(R,K+K',\tau)[1+n(R,K,\tau)]\} \qquad (4.9.8.)$$

where we have exploited the detailed form of $\underset{\sim}{L}^{>}$ (4.7.19.), the consistency conditions (II.54)-(II.57) and definition (II.20).

Therefore the transport theory determined by this chapter is characterised by the equations of motion (4.9.1.) and (4.9.2.) where the collision integrals are specified by electron-electron and electron-phonon scattering calculated through the expressions (4.9.6.)-(4.9.8.).

The general structure has the overall appearance of a Boltzmann-like equation except, in detail, the collision integrals are more complicated than we would otherwise expect due to the dynamic non-asymptotic nature of interactions. However the physical interpretation still exists as may be seen for example in the phonon collision integral (4.9.7.) where a phonon is scattered by knocking an electron into a previously empty state. The interaction between electron and phonon proceeds via a non-equilibrium dynamically screened interaction due to the intermediary interactions with the surrounding electron density. These interactions induce a dispersion in the allowed final energies of the scattered electron, hole and phonon which leads to the appearance of the spectral functions integrated over the energies Ω', Ω'', ω'. Moreover, because we are not dealing with asymptotic free states but dynamically evolving processes we do not consider a single collision has an infinite amount of time in which to approach a steady state before the occurrence of subsequent collisions. This leads to the finite time integral in all three collision terms which of course leads to energy conservation factors that are not precisely δ-function terms as a consequence of the uncertainty relations.

The spectral functions appearing in these collision integrals have been approximated in §4.6. where it was evident that a complicated non-linear dependence on the effective driving field was introduced into the collision integrals explicitly, and not just indirectly through the distribution functions. However we recognise that the spectral functions modify not only the energy conserving factors, but the effective interactions

themselves through the non-equilibrium screening function (4.7.27.). This interaction-field-effect is an unexplored phenomenon which is considered by various model situations in the next chapter but prior to these calculations we should indicate how the conventional Boltzmann equation is obtained from the suitable limits of our transport equations. To this end we consider only the electron plasma where our transport theory implies the equation

$$[\partial_T + \frac{P}{m}\cdot\partial_R + eE\cdot\partial_p]f(R,P,T) = \left.\frac{-\partial f}{\partial T}\right|_{e\text{-}e}$$

where $\partial f/\partial T\big|_{e\text{-}e}$ is given by (4.9.6.).

If we first consider the equation as describing infinite lifetime quasi-particles then the spectral functions collapse to δ-functions. Furthermore if we allow the asymptotic limit ($T \to \infty$) then the integral over τ in (4.9.6.) gives an energy conserving δ-function $2\pi\delta(\Omega' - \Omega'')$ in which case the collision integral is expressible as

$$\int d^3P'd^3P''d^3P''' \left|\frac{\phi(P''' - P')}{\epsilon(P''' - P', \epsilon(P''') - \epsilon(P'))}\right|^2$$

$$x \{f(P)[1 - f(P''')]f(P')[1 - f(P'')]$$

$$- [1 - f(P)]f(P''')[1 - f(P')]f(P'')\}$$

$$x \delta(P - P' - P'' + P''')2\pi\delta[\epsilon(P) - \epsilon(P') - \epsilon(P'') + \epsilon(P''')]$$

$$\equiv \int dP'[W(P,P')f(P) - W(P',P)f(P')] \qquad (4.9.9.)$$

where $W(P,P')$ denotes a transition rate from a state with momentum P to one of P' that is determined from the squared interaction matrix multiplied by the energy density of final states. This pair, (4.9.1.) with (4.9.9.) constitutes the conventional Boltzmann equations. It has been obtained from the quantum treatment under the assumptions of slowly varying distribution functions, infinite lifetime quasi-particles and asymptotic boundary conditions.

The latter two assumptions are equivalent to taking the collisions as instantaneous and point-like which allows each collision to be irreversibly completed before its' next collision event and of course it eliminates any explicit dependence of the collision integral on the effective field.

Thus to summarise this chapter, we have obtained a transport theory applicable to the medium small device in high electric fields characterised by transport equations of a Boltzmann-like form. The many body effects of electron-electron interactions act to produce non-equilibrium dynamically screened interactions and renormalised phonon frequencies and group velocities. The collision integrals are non-asymptotic allowing for the extended nature of collisions and are explicitly field dependent through the spectral functions which affects both the energy conservation factors and the screened interactions.

CHAPTER 5

THE FIELD DEPENDENT SCREENING FUNCTION

§5.1. Introduction

In the last chapter a transport theory was developed which is capable of describing electron-phonon dynamics in the semi-classical transition regime of sub-micron semiconductor devices between the currently manufactured devices describable in terms of classical dynamics and the conjectured future devices relying on fully quantum ballistic transport. The corresponding transport equations ((4.9.1.) and (4.9.2.) with (4.9.6.)-(4.9.8.)) epitomising this transition regime have features characteristic of classical transport theory combined with features, notably in the collision integrals, due to the small time scales representing the dynamic behaviour. Specifically because the physics of such a device is inherently non-asymptotic the collision integrals must take into account the finite extent of particle interactions which leads to the exhibited non-local form. Consequently the energy conserving δ-functions have to be replaced with spectral functions and the action of a driving field within the interaction event leads to an explicit field dependence in the collision integrals since the particles will acquire energy picked up from the field within an extended collision.

This phenomenon of an explicit field-dependent collision integral was first appreciated by Levinson[57] and later dubbed the "Intra-Collisional-Field-Effect" by Barker[8]. We can see from the explicit form of the collision integrals introduced in Chapter 4 that the intra-collisional-field-effect manifests itself in two distinct ways: first in a fashion analogous to the energy conserving δ-function factors in the Fermi Golden Rule and secondly these energetics act to modify the effective interactions through the screening functions' (4.7.27.) explicit dependence on the spectral function (4.6.29.). The first of these modifications has been the subject of much study over the past decade[11][12][30][40][41] to such

an extent that it alone has become synonymous with the intra-collisional-field-effect. Yet in spite of this research it still has not been conclusively determined how important this particular modification will be to the transport (for example see the recent papers of Herbert and Till[40][41]).

In contrast, this second aspect of the intra-collisional-field-effect has received very little attention to the point where it is presently completely unknown as to whether the field dependence of the effective interaction will have any significant effect whatsoever on the scattering rates.

Therefore this chapter is devoted to an analytic study of the interaction-field-effect by using several very simple models in order that calculations may be performed on the screening function (4.7.27.). It is to be hoped that this procedure in spite of the simple models will help to shed some light on the relative importance of this particular field effect. To this end we must first reduce the expression into a more recognisable form. Thus from the definition of the screening function (4.7.27.) combined with definitions (4.7.18.) and (4.7.19.) we have

$$\epsilon[RTP\omega] = 1-\phi(P)L(RTP\omega)$$

$$= 1-\phi(P)\int \frac{d\omega'}{2\pi}\frac{L^{>}(RTP\omega') - L^{<}(RTP\omega')}{\omega-\omega'}$$

$$= 1-\phi(P)\int \frac{d\omega'}{2\pi}\frac{d\omega''}{2\pi}\,dP'[G^{>}(RTP' + \tfrac{P}{2},\omega'' + \tfrac{\omega'}{2})G^{<}(RTP' - \tfrac{P}{2},\omega'' - \tfrac{\omega'}{2})$$

$$- G^{<}(\quad " \quad)G^{>}(\quad " \quad)]/\omega - \omega' \qquad (5.1.1.)$$

The above time-ordered one-electron Greens functions in (5.1.1.) may be converted into one-electron Wigner functions and spectral density functions by making use of the consistency conditions (II.54.) and (II.55.) which gives for the screening function:-

$$\epsilon[RTP\omega] = 1 - \phi(P) \int \frac{d\omega'}{2\pi} \frac{d\omega''}{2\pi} dP' \frac{[f(RTP' - \frac{P}{2}) - f(RTP' + \frac{P}{2})]}{\omega - \omega' + \omega''}$$

$$x \; a(RTP' + \frac{P}{2}\omega')a(RTP' - \frac{P}{2}\omega'') \qquad (5.1.2.)$$

This is an exact expression for the screening function in terms of one-electron quantities only limited by the approximations which were used in Chapter 4 to obtain the transport equations. Moreover, the electron spectral function is given explicitly by (4.6.29.) where it is seen that the function is explicitly dependent on the driving field through the field dependent variables (4.6.28.).

However this exact form of the screening function is far too complicated to attempt any analytical study because it involves the electron Wigner function, spectral function and effective driving field. In order to obtain the effective driving field and spectral function we require a knowledge of the Wigner function which in turn is determined from its' transport equation, which of course depends on the screening function. Therefore the difficulty arises because the calculation may only be performed self-consistently within the rest of the transport problem simultaneously. Hence in order to isolate the interaction-field-effect it is necessary to assume simple models to reduce the screening function to a more manageable form.

The first of these assumptions is to specify the functional variation of the spectral function with the field-dependent parameters $R_0P_0\omega_0$. The simplest choice we can make physically corresponds to a quasi-particle picture where the particles are taken to have infinite lifetimes. We can see from (4.6.29.) i.e.

$$a(RTP\omega) = \frac{\Gamma(R_0P_0\omega_0)}{[\omega_0 - \bar{\epsilon}(R_0P_0\omega_0)]^2 + [\frac{\Gamma(R_0P_0\omega_0)}{2}]^2} \qquad (5.1.3.)$$

where $\bar{\epsilon}$ is an effective energy which includes a contribution from the real part of the self energy and

$$R_0 = R - \int_0^T d\tau \frac{P}{m}$$

$$P_0 = P - \int_0^T d\tau eE(\tau)$$

$$\omega_0 = \omega + V_{eff}(T) - V_{eff}(0) \qquad (5.1.4.)$$

that the imaginary part of the self energy Γ corresponds to a spread in the energy dispersion relation which, in the infinite lifetime limit will tend to zero (from the uncertainty relation $\Gamma\tau \gtrsim \frac{\hbar}{2}$ [98]).

In which case (5.1.3.) is a representation of a δ-function i.e.

$$a(RTP\omega)\Big|_{\Gamma\to 0} = 2\pi\delta(\omega_0 - \bar{\varepsilon}(R_0P_0\omega_0)) \qquad (5.1.5.)$$

where $R_0P_0\omega_0$ are given in (5.1.4.). This is as we would expect for a non-interacting quasi-particle with energy $\bar{\varepsilon}$ - each momentum value uniquely determines the particle energy as demonstrated for free particle Greens functions in Appendix II.

Using assumption (5.1.5.) in (5.1.2.) yields a screening function which looks very much like the Lindhardt screening function used in certain linearised transport theories[39][60][72][83] i.e. we obtain

$$\epsilon[RTP\omega] = 1 - \phi(P) \int dP' \frac{[f(R,T,P' + \frac{P}{2}) - f(R,T,P' - \frac{P}{2})]}{\bar{\varepsilon}(R_0,\omega_0,P' + \frac{P}{2} - \int_0^T d\tau eE(\tau)) - \bar{\varepsilon}(R_0\omega_0P' - \frac{P}{2} - \int_0^T d\tau eE(\tau)) - \omega} \qquad (5.1.6.)$$

The differences are that (5.1.6.) is a non-equilibrium expression involving the electron Wigner distribution and is explicitly field dependent due to the finite collision durations which contribute to the carrier energies.

The next problem to be overcome concerns the effective driving field. Of course this is obtained from the effective potential which itself ought to be calculated from Poissons equation with extra source terms due to the local densities of electrons and phonons. As these can only be derived from their respective (coupled) transport equations we are again involved in a

complete self-consistent calculation. (These difficulties are indicative of the complexities involved in solving a particular transport problem even when we have approximate transport equations of motion.) However since our principal concern in this chapter is with the effect of a field acting within one collision event rather than attempting to follow the evolution across a device it should be a reasonable first approximation to assume that the driving field is constant (in time at least). Therefore if τ_E is a measure of the mean collision time, or perhaps more accurately the average time two particles may be considered to be correlated with the field during an interaction, then the contribution of the field to the carrier momentum within a collision event is just $eE\tau_E$. Order of magnitude calculations have been performed by Nougier[70] to estimate τ_E in specific circumstances, however we can obtain a lower estimate from the uncertainty relation as follows. If we consider a simple collision event in the rest frame of the scatterer then we may consider an approaching particle with a relative momentum P scattering with a momentum P + P' in the absence of any correlation with the effective field. Consequently a measure of the spread in energy associated with this relative velocity of approach P/m is just

$$\varepsilon(P + P') - \varepsilon(P')$$

Alternatively if the field is correlated to this collision for a time τ_E then the particle will scatter with a relative momentum of $P + P' + eE\tau_E$ giving a subsequent spread in the energy of

$$\varepsilon(P + P' + eE\tau_E) - \varepsilon(P' + eE\tau_E)$$

Subtracting the first from the second gives a measure of the spread in energy associated with <u>just</u> the action of the field which if we assume a quadratic energy-momentum dispersion relation is just

$$\Delta\varepsilon_E = \frac{P\cdot eE}{m}\,\tau_E \qquad (5.1.7.)$$

However in the spirit of the uncertainty relations we know that this spread in energy due to the field is related to the minimum lifetime of the field action (i.e. τ_E) through[98]

$$\Delta\varepsilon_E \geq \frac{\hbar}{2\tau_E} \qquad (5.1.8.)$$

Using (5.1.7.) in (5.1.8.) gives an absolute lower bound for the mean correlation time of the field with a collision event, i.e.

$$\tau_E = \sqrt{\frac{\hbar m^*}{2|P\cdot eE|}} \qquad (5.1.9.)$$

The result (5.1.9.) is as we would expect, since the time available for the field to act in a collision should decrease for an increasing velocity of separation and for an increase in the accelerating force of the field.

The time independent homogeneous limit of (5.1.6.) using the effective mass energy-momentum dispersion approximation gives a screening function even more akin to the Lindhardt form. We find

$$\epsilon[P,\omega,E] = 1 - \phi(P)\int dP'\,\frac{f(P'+P) - f(P')}{\varepsilon(P+P') - \varepsilon(P') - \hbar\omega_E - \hbar\omega} \qquad (5.1.10.)$$

where ω_E is an equivalent <u>field-induced</u> frequency given explicitly by

$$\omega_E = \sqrt{\frac{|P\cdot eE|}{2\hbar m^*}} \qquad (5.1.11.)$$

and we have also made use of (5.1.9.). (We have also changed units in (5.1.10.) so that we now exhibit the explicit $\hbar$ dependence. We retain this unit system for the rest of this chapter.)

Thus we see that by using a series of simple models the problem of studying the complicated exact screening function (5.1.2.) has been reduced to one involving a screening function of Lindhardt-like form (5.1.10.). As we will be interested in the static behaviour of (5.1.10.) the function to be analysed is $\epsilon[P,\omega = 0,E]$ which can be seen from (5.1.10.) is just

$\epsilon[P,\omega = \omega_E,E = 0]$. In actual fact the correspondence with the Lindhardt form is precise since the true screening function governing the transition rates (as can be seen from (4.9.5.)-(4.9.7.)) is $\epsilon[P,\omega + i\delta]$. The extra factor of $i\delta$ was introduced naturally in Chapter 4 because our initial value problem was constructed out of causal functions.

It is to be hoped that the drastic reduction accomplished in complexity by this series of assumptions will not detract from the physics of allowing a field to act within a collision event, especially since the approximations have been limited to model the screening function itself and not the action of the field on any particular screening function. Moreover the simplified form (5.1.10.) is still too complicated an expression and we can only obtain any analytic results by employing a limited class of distribution functions which is essentially exhausted by δ-functions and Gaussians.

§5.2. The three-dimensional screening function for a Maxwellian distribution

In the introduction to this chapter it was demonstrated how a sequence of approximations could reduce the complicated screening function introduced in Chapter 4 down to a much simpler one of Lindhardt form. In order to study the effects of an electric field on the screening it is necessary to specify the precise form of the distribution function which will be taken to be of Gaussian form in this chapter. That is to say we take the distribution function, as a function of energy, to be a Maxwellian, i.e.

$$f(E) = e^{-\beta(E-\xi)} \qquad (5.2.1.)$$

where $\beta = 1/k_B T$ and $e^{\beta\xi}$ is a normalisation factor. Throughout this thesis we will always attempt to normalise to the total (known) electron density (n) so that

$$n = \int dE \rho(E) f(E) \qquad (5.2.2.)$$

where $\rho(E)$ is the energy density of states which for a three-dimensional

electron gas with a quadratic energy-momentum dispersion relation is given explicitly by

$$\rho(E) = \frac{4\pi(2m)^{3/2}}{(2\pi\hbar)^3}\sqrt{E} \qquad (5.2.3.)$$

Using (5.2.3.) in (5.2.2.) gives the explicit expression for the normalisation factor

$$e^{\beta\xi} = \frac{n(2\pi\hbar)^3\beta\sqrt{\beta}}{2\pi\sqrt{\pi}2m\sqrt{2m}} \qquad (5.2.4.)$$

which ensures that the distribution function normalises bo the correct electron density.

Therefore with $e^{\beta\xi}$ given by (5.2.4.), the distribution function is represented by a Gaussian if we use the effective mass quadratic energy-momentum relation, i.e. we have

$$f(k) = e^{\beta\xi}e^{-\lambda k^2} \qquad (5.2.5.)$$

where

$$\varepsilon(k) = \hbar^2k^2/2m^* \quad \text{and} \quad \lambda = \hbar^2\beta/2m \qquad (5.2.6.)$$

Converting the generalised sum implicit in $\int dp'$ to a three dimensional integral and summing over electron spins we can use the effective mass approximation, the distribution (5.2.5.) and the definition of the electron wavevector $q = P/\hbar$ to express the screening function (5.1.10.) as

$$\epsilon[q,\omega] = 1 + \frac{\phi(q)4\pi me^{\beta\xi}}{(2\pi)^3\hbar^2q}\int_0^\infty dk \int_{-1}^{1} dx\, ke^{-\lambda k^2}\, x$$

$$x\left[\frac{1}{x + a/2k + \frac{m\omega}{\hbar kq}} + x + \frac{1}{a/2k - m\omega/\hbar kq}\right]$$

$$\equiv 1 + \frac{\phi(q)me^{\beta\xi}}{2\pi^4\hbar^2q}\int_0^\infty dk\, ke^{-\lambda k^2}\left[\ln\left|\frac{k+\alpha_+}{k-\alpha_+}\right| - \ln\left|\frac{k+\alpha_-}{k-\alpha_+}\right|\right] \qquad (5.2.7.)$$

where $\alpha_{\pm} = m\omega/\hbar q \pm q/2$.

Changing variables from k to t where $\lambda k^2 = t^2$ and integrating (5.2.7.) by parts, once, gives

$$\epsilon[q,\omega] = 1 - \frac{\phi(q)me^{\beta\xi}}{4\pi^2\hbar^2 q\lambda}\left[\int_{-\infty}^{\infty} dt\, \frac{e^{-t^2}}{t - A_+} - \int_{-\infty}^{\infty} dt\, \frac{e^{-t^2}}{t - A_-}\right] \qquad (5.2.8.)$$

where $A_{\pm} = \sqrt{\lambda}\alpha_{\pm} = x \pm \frac{a}{2}$ and

$$x = \sqrt{\frac{\beta m}{2}}\,\frac{\omega}{q} \qquad (5.2.9.)$$

$$a = \sqrt{\frac{\hbar^2 q^2 \beta}{2m}} \qquad (5.2.10.)$$

However from Appendix VI we recognise that (5.2.8.) involves the so called Plasma (Dispersion) Function Z(s) where

$$Z(s) = \frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty} dt\, \frac{e^{-t^2}}{t - s}$$

If we also take the bare Coulomb potential statically screened by the dielectric constant ϵ_∞ to be represented by

$$\phi(r) = e^2/4\pi\epsilon_\infty r$$

then its' Fourier transform is just

$$\phi(q) = e^2/\epsilon_\infty q^2 \qquad (5.2.11.)$$

Thus combining (5.2.4.) and (5.2.11.) in (5.2.8.) gives the model screening function in three dimensions using a Gaussian distribution (in momentum) of

$$\epsilon[q,\omega] = 1 + \left(\frac{\kappa_D}{q}\right)^2\left[\frac{Z(x - \frac{a}{2}) - Z(x + \frac{a}{2})}{2a}\right] \qquad (5.2.12.)$$

where κ_D is the same inverse Debye screening length (λ_D) often used in discussions of classical electron plasmas[72] and is given explicitly by

$$\kappa_D^2 = \frac{ne^2\beta}{\epsilon_\infty} \qquad (5.2.13.)$$

The expression (5.2.12.) is of central importance to this chapter since it represents a model screening function which may be used to analyse the field dependence (through ω and hence through the x-variable) of the effective interactions. However before we proceed with an analysis of our screening function, a few comments on its' various constituents are in order.

First the Plasma function is in general a complex function of complex argument and indeed we will be concerned with the values of Z(s) in the upper half complex plane. This is because the correct function governing the scattering behaviour is $\epsilon[q,\omega + i\delta]$ as previously indicated which means that at the very least the x-variable in the Plasma function must be considered to have a small imaginary component and Z(s) has to be evaluated in the limit of this component tending to zero. (This is <u>not</u> the case if we consider collisional damping in the model screening function since then the x-variable will have a finite imaginary part. This case will be treated later in section 5.4. (see also Appendix VIII).)

Secondly the dimensionless plasma parameters (x) and (a) have a direct physical interpretation since if we introduce the mean thermal velocity $\langle v \rangle$ and a corresponding thermal wavelength λ_T for the electrons through

$$\frac{1}{2} m\langle v \rangle^2 = \frac{1}{\beta} \qquad (5.2.14.)$$

and

$$\frac{\hbar^2 q_T^2}{2m} = \frac{1}{2m} (\hbar/\lambda_T)^2 = \frac{1}{\beta}$$

then we see that (5.2.9.) and (5.2.10.) have the more reasonable form

$$x = (\omega/q)/\langle v \rangle$$

$$a = q/q_T = \lambda_T/\lambda \qquad (5.2.15.)$$

Therefore the field-dependent x-parameter has the significance of the ratio

of the electrons' phase to its' thermal velocity, and "a" represents the ratio of thermal to kinetic wavelengths.

The appearance of thermal wavelengths and velocities, the Debye screening length and even the Plasma Dispersion function is not coincidental - they are all a consequence of employing the Gaussian distribution function in the Lindhardt-like screening function. This is not a particular detriment since we want to study the effects of a field on the screening rather than whether the model screening function is an accurate representation of the physics. However we can use the interpretation of the plasma parameters (5.2.15.) to show that our screening function (5.2.12.) has the correct classically limiting behaviour when compared with the conventional work on the statics and dynamics of an electron plasma as we now illustrate.

§5.3. Classical limit of the screening function

In the previous section a model screening function was obtained with the use of a Gaussian distribution function which involved a field-dependent variable x ($\propto \sqrt{E}$) and a variable "a" which was proportional to $\hbar$. Of course various screening functions have been used for many years in the discussions of classical transport behaviour with regard to the long range Coulomb interaction[56][60] and so we would expect that the classical limit of our screening function should reproduce an appropriate standard description. This section demonstrates that the suitable limit yields the Debye screening theory of a point charge and the same function is capable of describing some of the dynamics of such an electron plasma.

It is convenient to split the screening function (5.2.12.) into its' real and imaginary parts (recall we are concerned with $\lim_{\delta \to 0} \varepsilon[q,\omega + i\delta]$ by using the properties of the Plasma Function (Appendix VI) which furnishes us with

$$\mathrm{Re}\epsilon[q,\omega] = 1 + \left(\frac{\kappa_D}{q}\right)^2 \left[\frac{\mathrm{ReZ}(x - \frac{a}{2}) - \mathrm{ReZ}(x + \frac{a}{2})}{2a}\right] \qquad (5.3.1.)$$

and

$$\mathrm{Im}\epsilon[q,\omega] = \frac{\sqrt{\pi}}{2a}\left(\frac{\kappa_D}{q}\right)^2 [e^{-(x-\frac{a}{2})^2} - e^{-(x+\frac{a}{2})^2}] \qquad (5.3.2.)$$

The first interesting limit we consider is when we set the electric field equal to zero (hence x = 0). From (5.3.2.) we see that this means the screening function is entirely real and by using the properties in Appendix VI gives an expression for the real part as

$$\epsilon[q,E = 0] = 1 - \left(\frac{\kappa_D}{q}\right)^2 \frac{\mathrm{ReZ}\left(\frac{a}{2}\right)}{a} \qquad (5.3.3.)$$

This may be considered as a quantum generalisation of the standard Debye form (i.e. $\epsilon[q] = 1 + \left(\frac{\kappa_D}{q}\right)^2$) but where now the "screening length" is a q-dependent quantity. In fact the classical limit of (5.3.3.) may be obtained by using the power series expansion of the Plasma function (VI.5.),

$$\mathrm{ReZ}(s) \simeq -2s$$

which when substituted in (5.3.3.) yields precisely the Debye form. However the modifications incurred by this q-dependent screening are only slight in the physically interesting range of parameters as illustrated in figures (5.4.1.) and (5.4.2.). We will return to this point in the following section.

Note that the classical limit of (5.3.3.) which gives the usual Debye expression corresponds to point-like collisions in an electron plasma and is used to model the cuttoff in the infinite range of the Coulomb potential, since the 'bare' potential $\phi(q)$ is replaced by the screened form $\phi(q)/\epsilon(q) = e^2/q^2\epsilon[q] = e^2/q^2 + \kappa_D^2$ which has an inverse Fourier transform of $\phi_s(r) \propto \frac{e^{-r/\lambda D}}{r}$.

This last expression is indicative of the way the effect of the medium surrounding a point charge acts to alter the initial infinite range of the Coulomb potential ($\lambda_D \to \infty$) into one which decays exponentially over a distance

of the order of a Debye length. (Typically for $\epsilon_r = 13$ at a temperature of 300 K an electron density of 10^{16} cm^{-3} has a Debye length of order 430 Å compared to the interparticle spacing of 460 Å.)

Thus we see that for high density room-temperature systems our screening functions gives the correct limiting behaviour (in that it coincides with conventional Debye shielding). If we were concerned with low temperature degenerate systems we would perhaps prefer our screening function to reduce to the Thomas-Fermi theory[39][72] in which case we would start with the Fermi-Dirac function rather than the Maxwellian distribution, but this is another story.

In addition to reproducing the static Debye screening theory, we may use our screening function to analyse the effects of a uniformly moving test charge through a classical Maxwellian plasma as follows.

To obtain the classical limit we need the expansion of the Plasma Function for small (a) (since $a \propto \hbar$). Now since (Appendix IV)

$$Z(x + \tfrac{a}{2}) \simeq Z(x) + \tfrac{a}{2} Z'(x)$$

(5.2.12.) reduces to

$$\epsilon[\omega, q_{small}] = 1 - \left(\frac{K_D}{q}\right)^2 \frac{Z'(x)}{2}$$

and since we know the Plasma Function satisfies the differential equation (VI.4.)

$$Z'(x) = 2[1 + xZ(x)]$$

then the velocity dependent, classical screening function is just

$$\epsilon[q,\omega]\Big|_{classical} = 1 + \left(\frac{K_D}{q}\right)^2 [1 + xZ(x)] \qquad (5.3.4.)$$

Recall from (5.2.15.) that (x) bears the physical significance of the ratio of electron phase to thermal velocity and hence we should be able to use (5.3.4.) to study a uniformly moving test charge with a velocity of $u = x\langle v\rangle$

immersed in a classical Maxwellian electron plasma - perhaps the most extensively studied problem in plasma physics (for example see Wang et al.[95]).

The problem may be posed if we consider this test particle moving in the x-direction which, in the lack of a medium, will create the potential $V_x(r,t)$ given by solving Poissons equation

$$\nabla^2 V_x(r,t) = \frac{e^2}{\epsilon_\infty}\,\delta(r - ut)$$

or

$$V_x(k,\omega) = \frac{2\pi e^2}{\epsilon_\infty q^2}\,\delta(\omega - k\cdot u) \qquad (5.3.5.)$$

However with the inclusion of a surrounding plasma the effective potential is just $V_x(k,\omega)/\epsilon[k,\omega]$ which may be inverse Fourier-Laplace transformed using (5.3.4.) to give the real space effective potential produced by this moving test charge, i.e.

$$V(r,t) = \int \frac{dq^3}{(2\pi)^3}\int \frac{d\omega}{2\pi}\, e^{i(q\cdot r-\omega t)}\, \frac{2\pi e^2\delta(\omega - q\cdot u)}{\epsilon_\infty\{q^2 + \kappa_D^2\,[1 + xZ(x)]\}}$$

$$= \frac{e^2}{\epsilon_\infty(2\pi)^3}\int dq^3\, \frac{e^{iq\cdot(r - ut)}}{q^2 + \kappa_D^2[1 + xZ(x)]} \qquad (5.3.6.)$$

with $x = u/\langle v\rangle$.

Of course the Plasma Function is generally complex and (5.3.6.) must be evaluated numerically[95]. However the essential physics may be extracted if we ignore the imaginary part of the screening function (5.3.4.) which is only a reasonable assumption for small and large values of x as may be seen in the overleaf plot, Figure (5.3.1.) comparing the real and imaginary parts of the function $|1 + xZ(x)|$.

If we do neglect this imaginary component we see from (5.3.4.) that the screening function takes on a conventional form if we define a velocity-dependent screening length $\lambda_u (= 1/\kappa_u)$ by

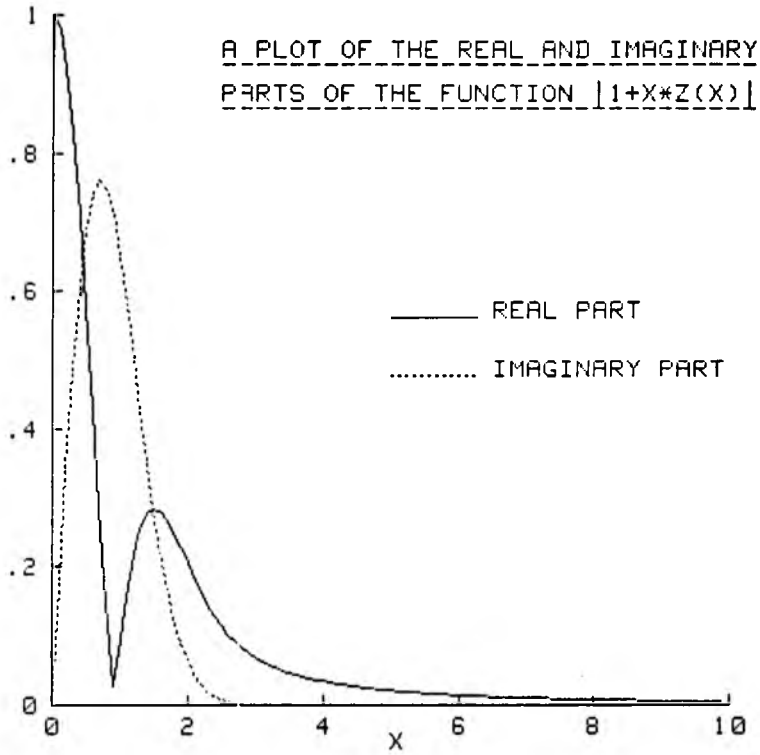

A PLOT OF THE REAL AND IMAGINARY
PARTS OF THE FUNCTION |1+X*Z(X)|
REAL PART
IMAGINARY PART
1
.8
.6
.4
.2
0
0
2
4
6
8
10
X

Fig. 5.3.1.

$$\lambda_u^2 = \frac{\lambda_D^2}{\mathrm{Re}(1 + xZ(x))} \qquad (5.3.7.)$$

in which case the effective potential (5.3.6.) becomes

$$V(R) = \frac{e^2}{\epsilon_\infty (2\pi)^2} \int_0^\infty dq \int_{-1}^{1} d\mu \, \frac{q^2 e^{iqR\mu}}{q^2 + \kappa_u^2}$$

$$= \frac{e^2}{4\pi\epsilon_\infty iR} \int_{-\infty}^{\infty} dq \, \frac{q e^{iqR}}{q^2 + \kappa_u^2} \qquad (5.3.8.)$$

where $R = r - ut$.

From (5.3.7.) and the behaviour of $1 + xZ(x)$ we note that κ_u^2 is positive for small values of x and negative for large values. Therefore if we first consider the situation when κ_x^2 is positive, then the integrand in (5.3.8.) has poles in the complex plane at $q = \pm i\kappa_u$ and closing the integration contour in the upper half plane gives the result for the effective potential of

$$V(r - ut) = \frac{e^2}{4\pi\epsilon_\infty} \frac{e^{-R/\lambda_u}}{R} \qquad (5.3.9.)$$

This is of the conventional Debye screened potential form but where now the screening length is a function of the velocity and since $1 + xZ(x)$ decreases with increasing velocity (as long as $x < 1$) this new screening length is greater than the Debye length. (If the test particle has zero velocity then (5.3.9.) is just the usual result of course.) Since this is only really valid for small x we may use the polynomial expansion of the Plasma Function (VI.5.) to show that the screening length should increase like

$$\lambda_u \simeq \lambda_D(1 + 2x^2)$$

that is, with the square of the test particle velocity. However, taking (5.3.7.) as it stands and using Figure 5.3.1., we can see that this screening length diverges when the test particle velocity is of the same order as the mean thermal velocity (i.e. $x \sim 1$). For greater test velocities λ_u^2 becomes negative and the concept of a screening length has broken down, in which case

we must return to (5.3.8.) and consider the situation for large x when κ_u^2 is negative. This now produces two poles on the real axis of $q = \pm|\kappa_u|$ and so deforming the integration contour to close in the upper half plane and pass just below the poles gives the different result for the potential

$$V(r - ut) = \frac{e^2}{4\pi\epsilon_\infty} \frac{\cos|\kappa_u|R}{R} \qquad (5.3.10.)$$

Since this is appropriate for large x we can use the asymptotic expansion of the Plasma Function (VI.6.) to show that

$$\kappa_u\Big|_{u>><v>} = \frac{\kappa_D}{\sqrt{2}} \frac{<v>}{u} = \frac{\omega_p}{u} \qquad (5.3.11.)$$

where we define a characteristic plasma frequency[72] by

$$\omega_p = \frac{\kappa_D <V>}{\sqrt{2}} = \sqrt{\frac{ne^2}{\epsilon_\infty m}} \qquad (5.3.12.)$$

Substituting (5.3.11.) in (5.3.10.) shows that the potential created by a fast moving particle is proportional to $\frac{\cos(\omega_p R/u)}{R}$ which is essentially a bare Coulomb modulated by an oscillating periodic function of wavelength $2\pi u/\omega_p$.

In fact if we retain the next order term in the asymptotic expansion of the plasma function we can obtain an approximate dispersion relation for the frequency since from

$$-\kappa_u^2 = \kappa_D^2[1 + x\mathrm{Re}Z(x)]$$

and $$\mathrm{Re}Z(s)\Big|_{s>>1} \simeq -\frac{1}{s}\left(1 + \frac{1}{2s^2} + \frac{3}{4s^4}\right) \qquad (VI.6)$$

we have that

$$\omega^2 = u^2\kappa_u^2 = \omega_p^2\left[1 + \frac{3}{2}\left[\frac{<V>}{u}\right]^2\right] \qquad (5.3.13.)$$

which has the same dependence used in conventional theory (for example see Lifschitz and Pitaevski §32[58]) for high frequency waves.

We also note that in the limit of extremely high test particle velocities $1 + xZ(x)$ tends to zero, the screening function is unity and the effective potential is of a bare Coulomb form.

All the foregoing results are consistent with a description of the electron gas established many years ago (see for example Pines[72]) which we may summarise briefly as follows. Firstly a stationary test charge immersed in a Maxwellian plasma effectively interacts with other particles not by the Coulomb interaction but by a shielded Coulomb potential which drops off exponentially over a finite distance called the Debye length. If the test charge is moving through the plasma at a slow velocity (less than the thermal velocity) then the screening cloud surrounding the particle is distorted along the direction of motion. The distance over which the potential exponentially decays is now greater than the Debye length and increases with the square of the particle velocity (from (5.3.9.)). At a critical velocity around the mean thermal velocity the plasma cannot react quickly enough to shield the test particle which essentially outruns its' screening cloud. For larger values of the particle velocity the resulting effective potential is long range and oscillating with a characteristic frequency ω_p(5.3.12.) and wavelength $2\pi u/\omega_p$. This produces the so called plasma oscillations in an electron gas which are collective oscillations of the electron density that can only be induced by long range correlations.

This interpretation is somewhat complicated due to the presence of the imaginary part of the Plasma function particularly at intermediate velocities which acts to damp the plasma oscillations and modulate the screened potential, where the damping will decrease as the velocity increases (as can be seen from Figure 5.3.1.). Note that this damping has nothing to do with the energy loss due to collisions but has, as its' source, a collisionless mechanism of energy dissipation first noted by Landau[55].

An intuitive description of this Landau damping has been given by Wu[100] and Dawson (see also Appendix B in "Plasma Kinetic Theory"[67]) as a resonant

power absorption of those particles travelling with the phase velocity of a plasma oscillation (and therefore damping should be most pronounced for the phase velocity around the thermal velocity which again is borne out in Figure 5.3.1.) although the difinitive argument appears to have been given by Rowlands[6][80] using a phase-mixing description. We will meet this phenomenon of Landau damping later in this chapter when we consider the explicit field dependence of the interaction which would be divergent were it not for this physically important process.

As a final comment of this section we remark that although this discussion has been concerned with a test particle velocity, we have equally well been concerned with the semi-classical limit of the interaction-field-effect since the particle velocity (ω/q) may be considered to be field-induced due to the explicit field dependence of the frequency (5.1.11.). In which case the phenomena mentioned in this section can be thought of as being due to the additional velocity acquired by the particle within a collision event from the extra energy picked up from the field. The magnitude of the electric field that could cause an appreciable effect will be discussed in the final parts of this chapter but the consideration of these semiclassical models indicate that the electric field will in general act to de-screen the interactions.

This section has exhausted the various limits of our screening function (5.2.12.) which allows us to extract analytically a simple description of the relevant physical behaviour of the electron system. Therefore we must now proceed to a numerical study of the effects an electric field acting within a collision may have on the interactions, including the imaginary part of the screening function.

§5.4. The Interaction-Field-Effect

In §5.2. the general screening function (5.1.2.) was reduced to a model form (5.2.12.) which was demonstrated in §5.3. to show a sensible limiting behaviour. This model screening function is seen to be controlled by the

ratio of electron phase to thermal velocities and kinetic to thermal wavelengths, where the electron phase velocity is due to a field induced frequency

$$\omega_E = \sqrt{\frac{eEq|\cos\theta|}{2m^*}} \qquad (5.4.1.)$$

It may be seen that the field effect depends not only on the magnitude of the electric field, but the momentum transfer $\hbar q$, the angle between the field and this momentum transfer θ and the effective mass of the electron - the effect being larger for small effective mass systems.

Consequently the field-effect will be most pronounced in low effective mass semiconductors like InSb and GaAs as opposed to Si, which is why we will use parameters applicable to electrons in the central conduction valley of GaAs in the numerical studies of this section.

We are thus in a position to address the question posed at the beginning of this chapter: to what significant extent will a strong electric field acting within a collision duration alter the effective interaction between particles (and consequently alter the transition rates)?

Hopefully the results of this section will shed some light on this particular aspect of the intra-collisional-field-effect. First however we need to decide what function has the most physical relevance since in the last section we saw how the concept of a screening length became meaningless for large velocities (and consequently for high electric fields). This is provided by the equations of motion obtained in Chapter 4 where it may be seen that the quantity altering the transition ratio through the effective interactions is just $1/|\epsilon[q,\omega_E + i\delta]|^2$. Therefore we would like to examine the real and imaginary parts of our model screening function for arbitrary wavevector values and a variety of electric field strengths, and moreover explore its' sensitivity to varying the system parameters such as temperature and electron density.

However we already have a variety of screening functions we could compare ranging from unity (corresponding to no screening at all) to a field-

dependent, wavevector-dependent quantum screening function (5.2.12.). The following diagram, Figure (5.4.1.), illustrates the relationships between the various screening functions where

$$\epsilon[q,\omega_E] = 1 + \left(\frac{\kappa_D}{q}\right)^2 \left[\frac{Z(x - \frac{a}{2}) - Z(x + \frac{a}{2})}{2a}\right] \qquad (5.4.2.(a))$$

$$\epsilon[q,\omega_E]\Big|_{\text{classical}} = 1 + \left(\frac{\kappa_D}{q}\right)^2 [1 + xZ(x)] \qquad (5.4.2.(b))$$

$$\epsilon[q,\omega_E]\Big|_{E=0} = 1 + \left(\frac{\kappa_D}{q}\right)^2 \frac{|\mathrm{Re}Z\left(\frac{a}{Z}\right)|}{a} \qquad (5.4.2.(c))$$

and $$\epsilon[q]\Big|_{\text{classical}} \equiv \epsilon[q \to 0, \omega_{E=0}] = 1 + \left(\frac{\kappa_D}{q}\right)^2$$

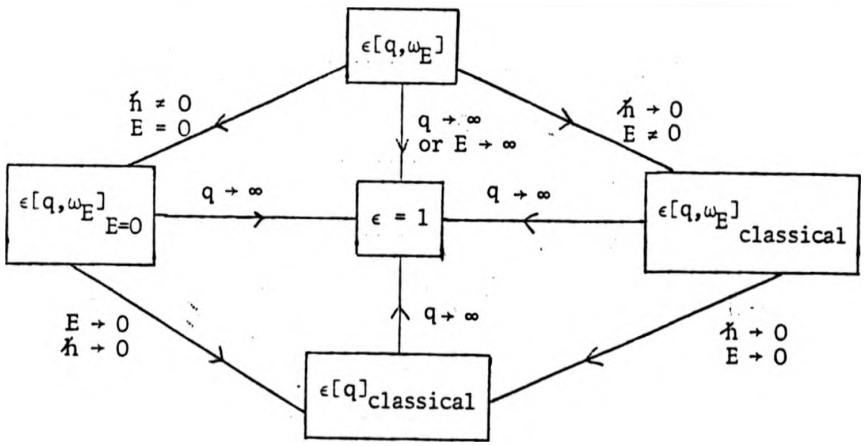


Fig. 5.4.1.

Limiting relationships between the model screening functions

Traditionally the Debye screening function (5.4.2.(d)) has been considered sufficiently accurate even to model the quantum transport of hot electrons in semiconductors[46][61] and thus the transition rates are governed by the square of the screened interaction

$$|\phi(q)/\epsilon[q]_{\text{classical}}|^2 \propto \left|\frac{1}{q^2 + \kappa_D^2}\right|^2 .$$

However as noted in §5.3. a better screening function would have a q-dependent screening length as indicated by (5.4.2.(c)) which would give modified transition rates dependent on

$$|1/(q^2 + \kappa_D^2 \frac{\left|\text{ReZ}\left(\frac{a}{2}\right)\right|}{a})|^2.$$

Therefore in order to examine the deviations incurred by the use of the Debye screening function as opposed to a 'static, quantum' screening function we will first examine the ratio of the 'correctly' screened potential to the Debye shielded potential, i.e. we are concerned with

$$\left|\frac{\phi_{(\text{Quantum screened})}}{\phi_{(\text{Debye screened})}}\right|^2 \equiv \left|\frac{q^2 + \kappa_D^2}{q^2 + \kappa_D^2|\text{ReZ}\left(\frac{a}{2}\right)|/a}\right| \qquad (5.4.3.)$$

Figure (5.4.2.) overleaf, is a plot of this ratio (5.4.3.) as a function of the wavevector (measured in units of the optic phonon wavevector in GaAs) for various typical values of the electron concentration to be found in devices. The diagram after this, Figure (5.4.3.), is a plot of the same ratio but where now its' sensitivity to temperature is illustrated.

As a computational note the diagrams in this section rely on evaluating the real part of the Plasma Function for at least one hundred arguments in each picture. Therefore in order to reduce computing time a (1/2) Padé approximant to the Plasma Function is used which is derived in Appendix VI. i.e. the Plasma Function is approximated by the ratio of two polynomials such that

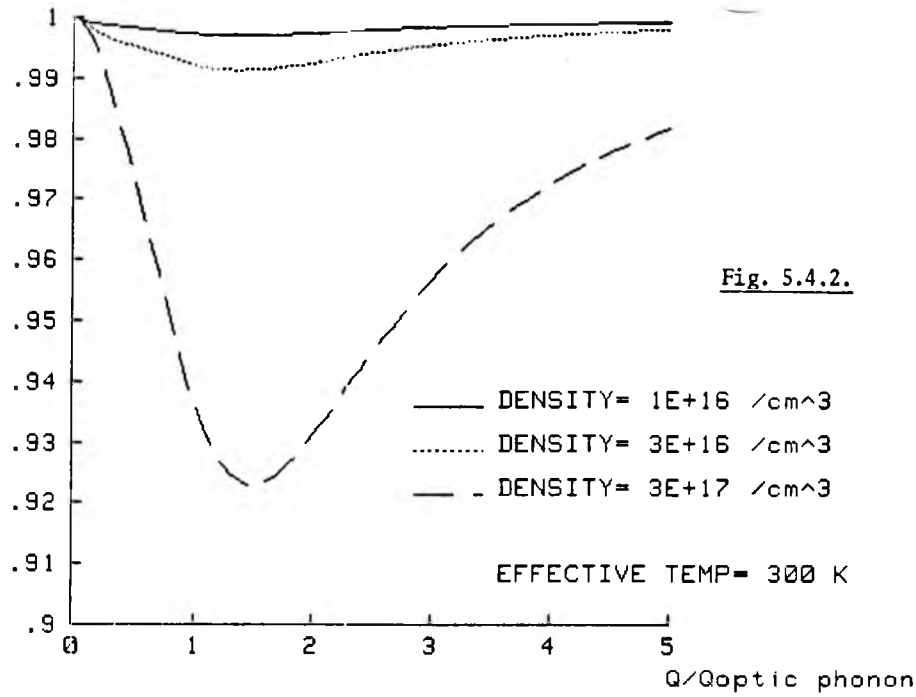


Fig. 5.4.2.

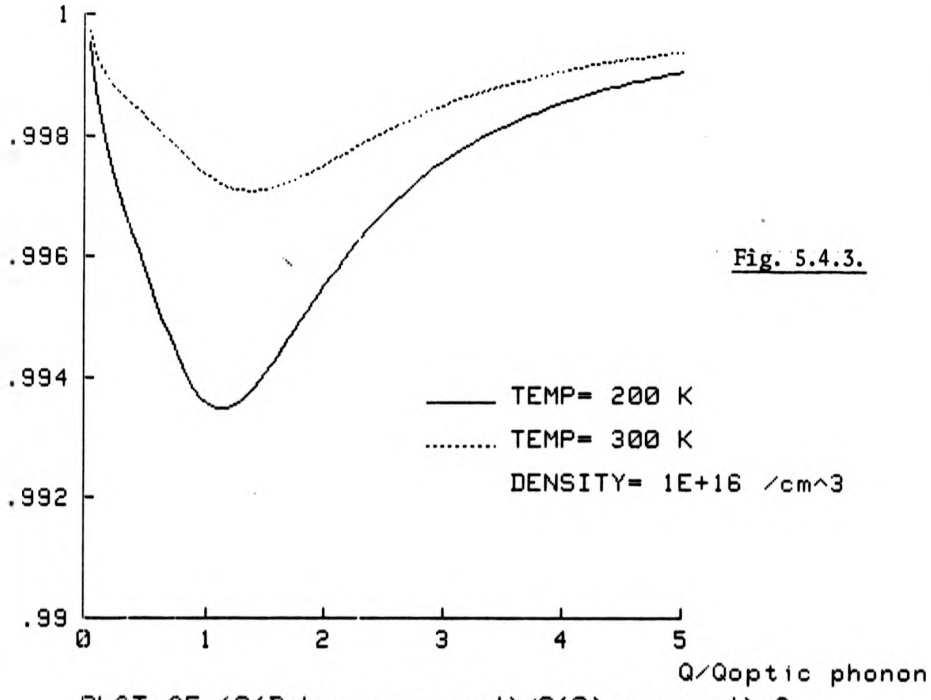


Fig. 5.4.3.

$$Z(s) = \frac{p_0 + p_1 s}{1 + q_1 s + q_2 s^2}$$

where the coefficients p_0, p_1, q_1, q_2 are generally complex numbers and are determined explicitly by four conditions related to the exact Plasma Function. The accuracy of this approximation may be gauged by examining the picture given in Appendix VI.

The qualitative behaviour of these figures is easily explained from (5.4.3.). We have already commented in §5.3. that in the semiclassical ($\hbar \to 0$) limit, expression (5.4.2.(c)) reduces to the classical Debye form and so the ratio represented by (5.4.3.) will in the long wavelength ($q \to 0$) limit always tend to unity independent of any variation of parameters. Similarly in the large q limit we may use the asymptotic expansion of the plasma function to show that both screening functions (5.4.2.(c)) and (d) will tend to unity, the first as $1/q^4$ and the second as $1/q^2$, and so their ratio, in the large q limit will also tend to unity as we observe in the figures. Moreover for a general q-value since $|\mathrm{Re}Z(a/2)|/a$ is a positive quantity, the ratio will be less than unity as is also seen. However, what is perhaps surprising is that the quantum screening function is so close to the Debye screening function, particularly in the physically interesting range of parameters indicated in the figures, that the scale of the axes must be so exaggerated that the pictures exhibit any variation whatsoever. (On a y-scale of 0 to 1 the lines in these figures are completely indistinguishable to the naked eye.) In fact from Figure (5.4.2.) even up to a room temperature density of 3×10^{17} electrons cm^{-3} the maximum difference is less than 8% and this occurs at one-and-a-half times the optic phonon wavevector where additional scattering mechanisms, not considered here, should act to reduce the electron concentrations at large momentum transfers and thus reduce the overall effect. The main conclusion from Figure (5.4.3.) is that the temperature of this ratio is not considered to be significant in comparison since a temperature drop of 100 K induces a change of no more than 0.4%

Therefore having determined that the use of a q-dependent screening length is of little improvement over the Debye screening length we can now examine the effects produced in the interaction by allowing the screening to deform due to the presence of an electric field within the collision process. To this end we consider the squared ratio of the field dependent effective potential, to the equivalent field independent potential, i.e. we consider

$$\left|\frac{\phi[q,\omega_E]}{\phi[q,\omega_E = 0]}\right|^2 = \left|\frac{q^2 + \kappa_D^2 |\mathrm{Re}Z(a/2)|/a}{q^2 + \kappa_D^2[Z(x - \frac{a}{2}) - Z(x + \frac{a}{2})]/2a}\right|^2 \qquad (5.4.4.)$$

and since $\epsilon[q,\omega_E = 0]$ is little different to the Debye form this ratio is a good indication of the differences that should be considered in conventional calculations that utilise Debye screening.

Obviously the zero field limit of (5.4.4.) gives a value of unity and hence if we plot the ratio (5.4.4.) against the momentum transfer wavevector for various values of the electric field strength, any effects explicit with the interaction-field will be exhibited by a departure from unity - if the ratio is greater than unity then the field induced interaction is greater than the field independent case and visa-versa. Figure (5.4.4.) overleaf is the first of such plots for a relatively low field range between 10 and 100 V cm^{-1}.

As can be seen, significant field effects occur for small momentum transfers, so for clarity this region is magnified and plotted in (5.4.5.).

In fact the ratio diverges as $q \to 0$ as can be seen from the diagram. This completely unexpected behaviour may be explained by examining the limits of the Plasma Function. We have previously seen (in §5.3.) that the $q \to 0$ limit of the field dependent screening function reduces to the classical field dependent form (5.4.2.(b)) which is governed by the function $1 + xZ(x)$, the real and imaginary parts of which are plotted in Figure (5.3.1.). Now if the field is zero then x is zero for all values of q and

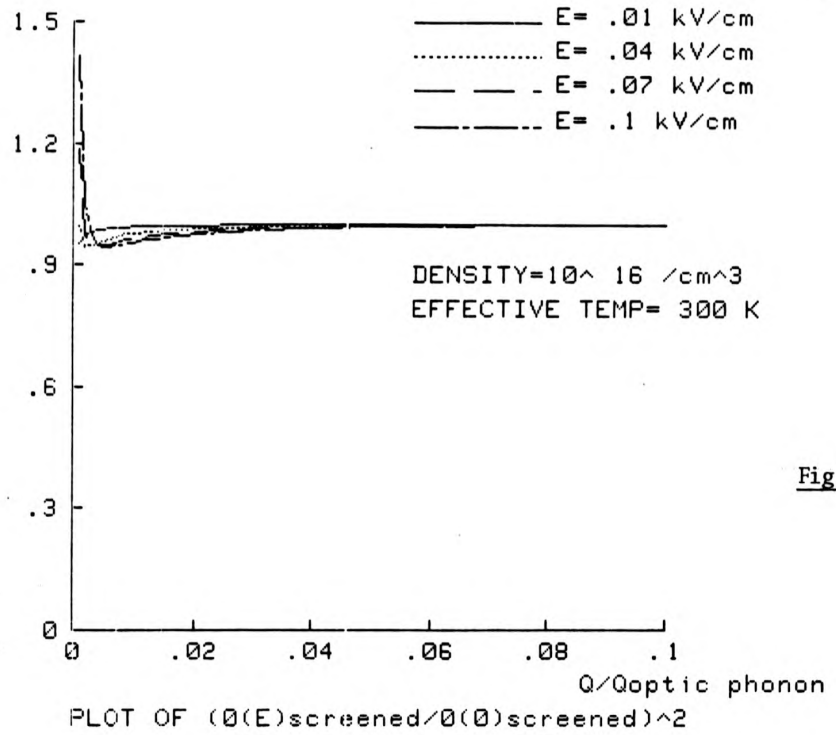


Fig. 5.4.4.

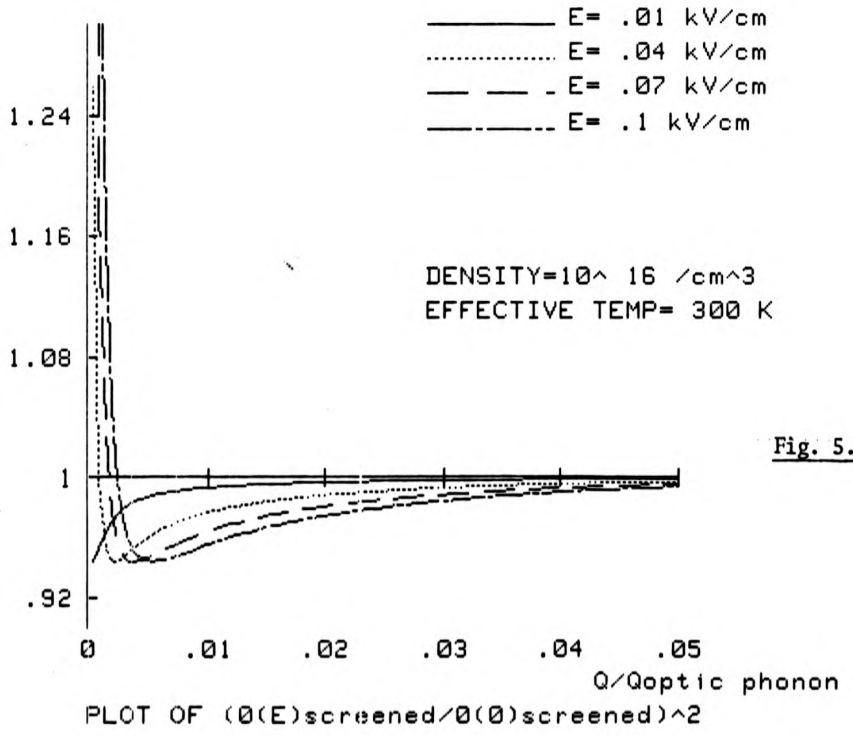


Fig. 5.4.5.

the screening function is of a simple Debye form. However for any non zero electric field, x will vary as $1/\sqrt{q}$ and hence will diverge as $q \to 0$. In which case $1 + xZ(x)$ will tend to zero leaving a residual screening function of unity so that the ratio (5.4.4.) in the limit of small q will behave like $1/q^4$ and so diverges, just as we observe.

It is possible to relate this divergence to a well known problem in studies of the dielectric function[39] where it is recognised that one must be careful in obtaining $\epsilon[0,0]$ in which order one allows $(q,\omega) \to 0$ since in general the two limits $\epsilon[q,0]\big|_{q\to 0}$ and $\epsilon[0,\omega]\big|_{\omega\to 0}$ will be different. This phenomenon is precisely what we observe in Figure (5.4.5.) and may be traced back to the ambiguity of the phase velocity in the two limits: if the field is zero then ω_E is also zero and the phase velocity is zero irrespective of q. However for a non zero electric field the phase velocity diverges as $q \to 0$ thus exhibiting a markedly different behaviour in the two limits of ($\omega = 0$, $q \to 0$) and ($q = 0$, $\omega \to 0$). This is an excellent example of why the inclusion of the intra-collisional-field-effect should produce non-standard type behaviour in transport calculations.

We would anticipate that this explicit interaction-field-effect will be exaggerated as we go to higher field strengths which is precisely what we see in the following two pictures, Figures (5.4.6.) and (5.4.7.) which plot the same ratio of the same value of temperature and electron density but for field strengths in the range of 0.1 to 10 kV cm^{-1}.

It is plain to see, particularly from Figure (5.4.7.), that our model predicts a significant interaction-field-effect in high electric field strengths for wavevector values up to one tenth the way towards the optic phonon wavevector. Before we comment on this further, we should really analyse the sensitivity of these deviations to the physical parameters such as density and temperature.

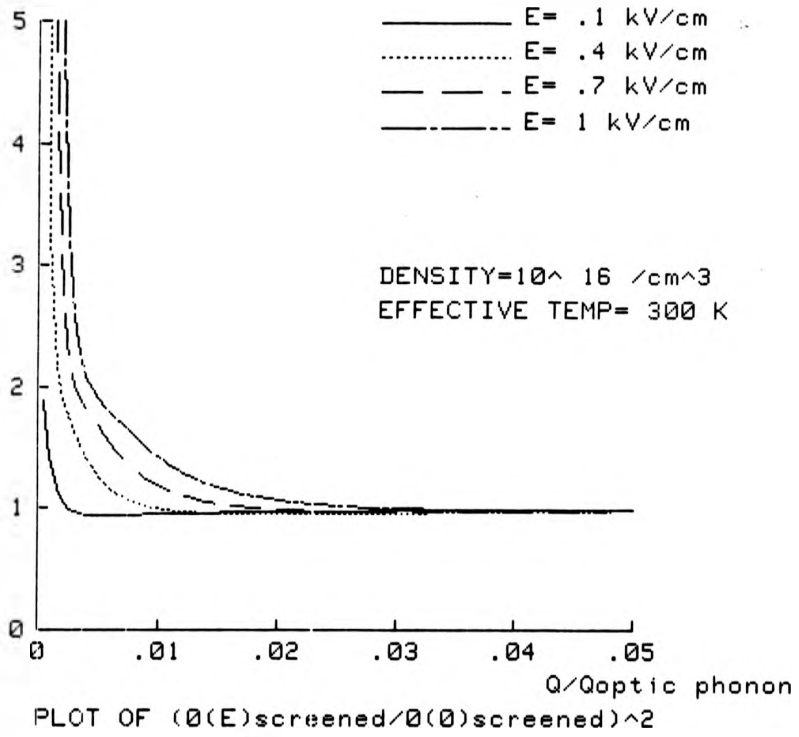

E= .1 kV/cm
E= .4 kV/cm
E= .7 kV/cm
E= 1 kV/cm
DENSITY=10^ 16 /cm^3
EFFECTIVE TEMP= 300 K
5
4
3
2
1
0
0
.01
.02
.03
.04
.05
Q/Qoptic phonon
PLOT OF (0(E)screened/0(0)screened)^2

Fig. 5.4.6.

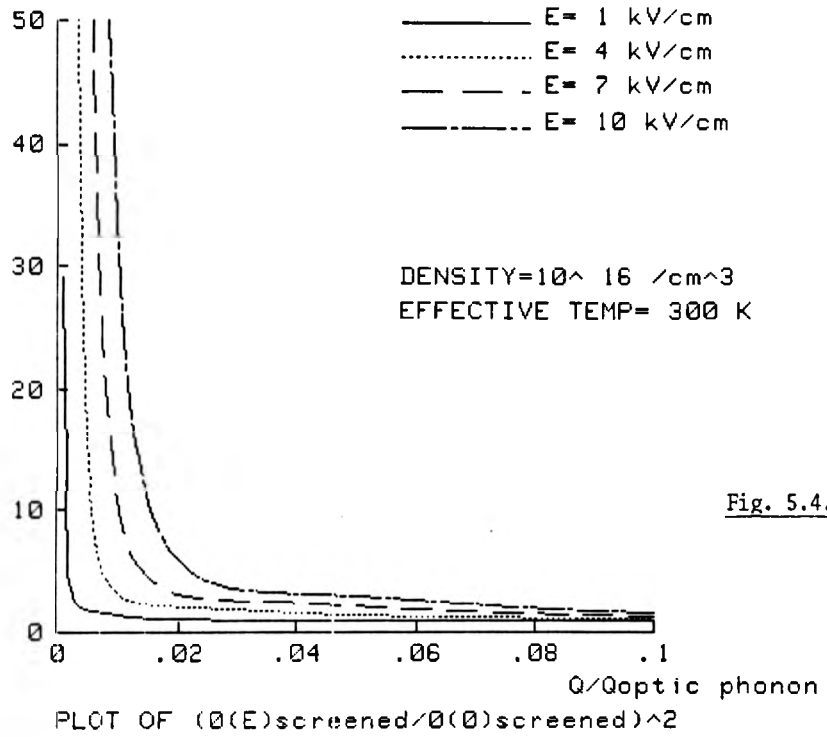


Fig. 5.4.7.

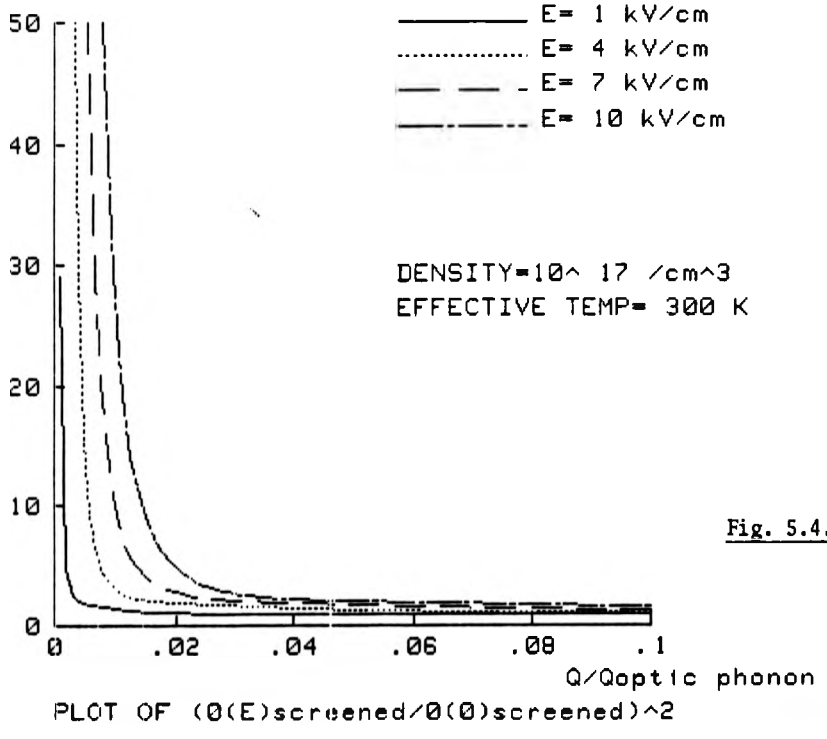


Fig. 5.4.8.

In particular if we consider an equivalent system but with a higher electron density, the plasma should be more efficient at screening a particular charge and the system Debye length will be reduced. Therefore for a given magnitude of electric field the energy picked up within a collision will be reduced for larger electron densities and thus larger fields would be required to produce the same effect. These deductions are the content of the next picture Figure (5.4.8.) which corresponds to Figure (5.4.7.) but with an increased electron density of 10^{17} cm^{-3} where we can see that although the density does alter the effect, it is not a particularly striking reduction.

Unfortunately the divergence at small q does much to distort the true interaction field effect in these pictures because we chose to compare against the Debye screening function and of course the action of a large field destroys the Debye form of the screening. Consequently it would perhaps be a more realistic choice to compare the field dependent screened interaction to the bare Coulomb potential since then the resulting pictures would include correlation effects due to the full screening of the electron plasma plus the descreening effects of the electric field. Therefore we are now concerned with the study of the ratio

$$\left|\frac{\phi[q,\omega_E]}{\phi[\text{Bare Coulomb}]}\right|^2 = \left|\frac{q^2}{q^2 + \kappa_D^2[Z(x - \frac{a}{2}) - Z(x + \frac{a}{2})]/2a}\right|^2 \qquad (5.4.5.)$$

This function does not diverge anywhere since in the limit of small q it will vary depending on

$$1 + \left(\frac{\kappa_D}{q}\right)^2 [1 + xZ(x)]$$

which diverges with 1/q as may be seen from the asymptotic expansion of Z(x) (VI.6.) and using the q-dependent form of the x-variable ((5.2.15.) and (5.4.1.)). Therefore the inverse of this function governing the ratio (5.4.5.) will tend to zero as q tends to zero irrespective of the electric

field. For large q both numerator and denominator increase with q^2 and so their ratio will tend to unity in this limit.

Before we consider the numerical plots of (5.4.5.) it is helpful to put the pictures in perspective by bearing in mind that the value of unity in the figures means the screened potential is equal to the bare Coulomb potential.

Thus the first of the plots of (5.4.5.), Figure (5.4.9.), corresponds to an electron concentration of 10^{16} cm^{-3} at a temperature of 300 K for a range of high field values between 2 and 20 kV cm^{-1}.

This Figure depicts the limiting behaviour we expected from analytic considerations of (5.4.5.) of small and large q for all field values. The bottom curve in Figure (5.4.9.) is a reasonable approximation to the curve we would have obtained if we had plotted the ratio of the Debye screened potential to the bare Coulomb potential. Therefore we note that in all field-dependent curves the screened potential is <u>greater than</u> the classically expected form which is further corroboration that the electric field acts to descreen the interaction.

As we have already illustrated between Figures (5.4.7.) and (5.4.8.) an increase in density will tend to reduce the field-effect apparent in (5.4.9.), but equivalently a <u>decrease</u> in the electron concentration should enhance this phenomenon. Thus although the typical doping densities in small devices are greater than 10^{16} cm^{-3}, the next two diagrams show the behaviour of this field effect as we reduce this concentration to 5×10^{15} cm^{-3} and 3×10^{15} cm^{-3} respectively.

The reason for considering the behaviour at lower densities is obvious from these two diagrams since a completely unexpected behaviour occurs at sufficiently high electric fields which may be summarised as follows: since the value of unity represents the bare Coulomb potential we see that Figures (5.4.10.) and (5.4.11.) are evidence that for a range of momentum transfers depending on the field strength, the 'screened' potential is actually <u>greater</u>

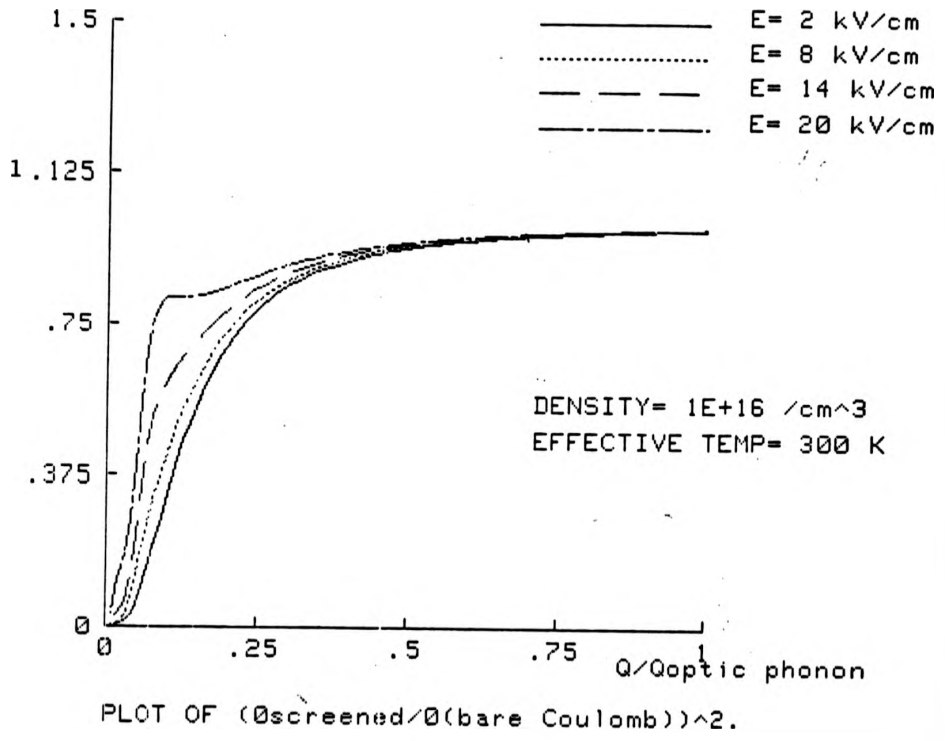

1.5
1.125
.75
.375
0
0
.25
.5
.75
1
Q/Qoptic phonon
E= 2 kV/cm
E= 8 kV/cm
E= 14 kV/cm
E= 20 kV/cm
DENSITY= 1E+16 /cm^3
EFFECTIVE TEMP= 300 K
PLOT OF (Øscreened/Ø(bare Coulomb))^2.

Fig. 5.4.9.

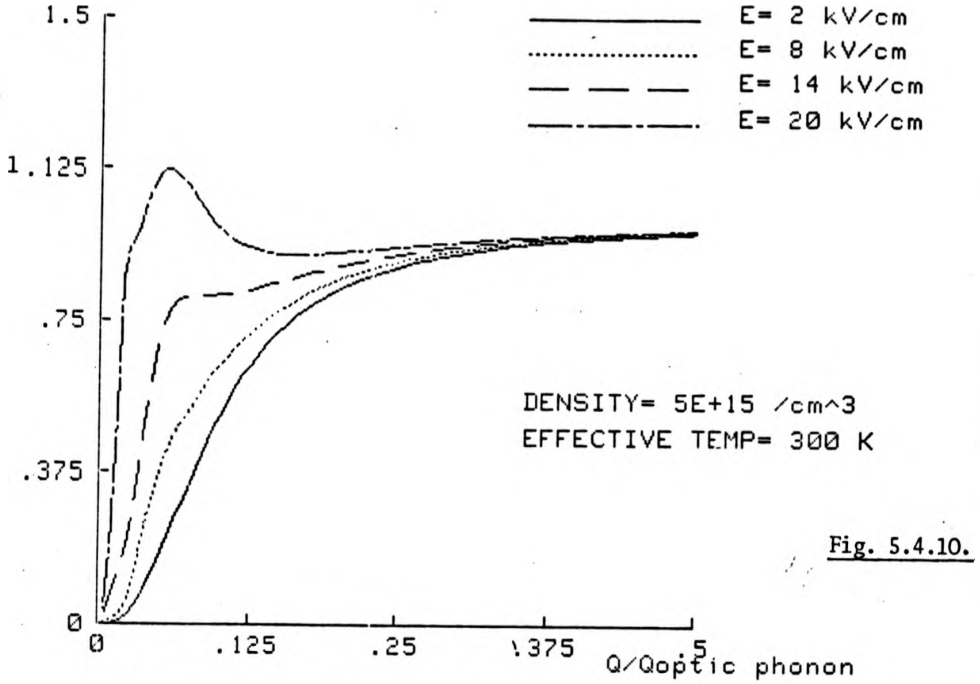


Fig. 5.4.10.

PLOT OF (Øscreened/Ø(bare Coulomb))^2.

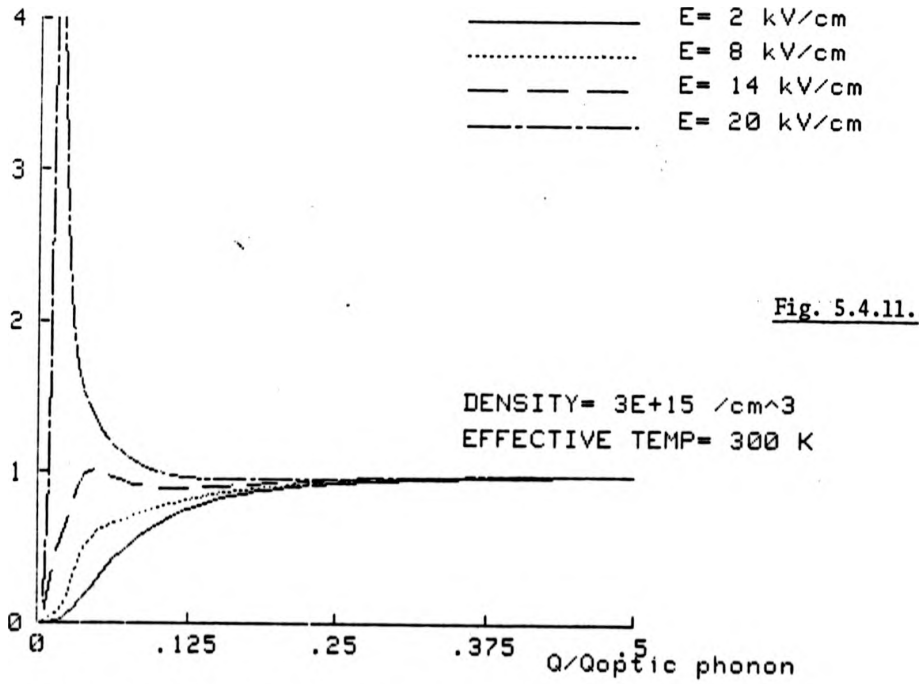


Fig. 5.4.11.

PLOT OF (Øscreened/Ø(bare Coulomb))^2.

than the original bare Coulomb interaction. This is a phenomenon entirely peculiar to the action of the electric field within a collision event. It has previously been anticipated that a strong electric field can act to descreen the effective interaction but the previous pictures indicate that it is possible to not just de-screen the potential but to enhance, or anti-screen, the interaction.

The implications and consequences of such a peculiar reaction remain uninvestigated at this time.

Of course a further product of the interaction field effect is that because it depends on the component of the electric field along the momentum transfer vector (see (5.4.1.)) we should see a marked inhomogeneity in direction of the transition rates as a consequence of angular variations of the screening function. In order to exhibit this dependence we use the angular dependence of the field-induced frequency (5.4.1.) in the ratio (5.4.5.) and plot this function against the angle between field and momentum transfer. The corresponding polar plot is given in Figure (5.4.12.) where we use an electron concentration of 10^{16} cm^{-3} at 300 K and a particular momentum transfer of one tenth the optic-phonon equivalent. Therefore Figure (5.4.12.) corresponds to the angular variation of Figure (5.4.9.) taken at a cross-section value of 0.1.

As can be seen there is no interaction field effect for momentum transfers perpendicular to the field of course which is why we expect this apparent directional inhomogeneity - the maximum effect being produced along the field direction.

At this stage it is perhaps useful to give an interim account of what has been accomplished so far in this section: we have obtained figures depicting the interaction-field-effect and examined its' variations with respect to the electron concentration, temperature, angle between field and momentum transfer and of course with the magnitude of the electric field in a three dimensional plasma.

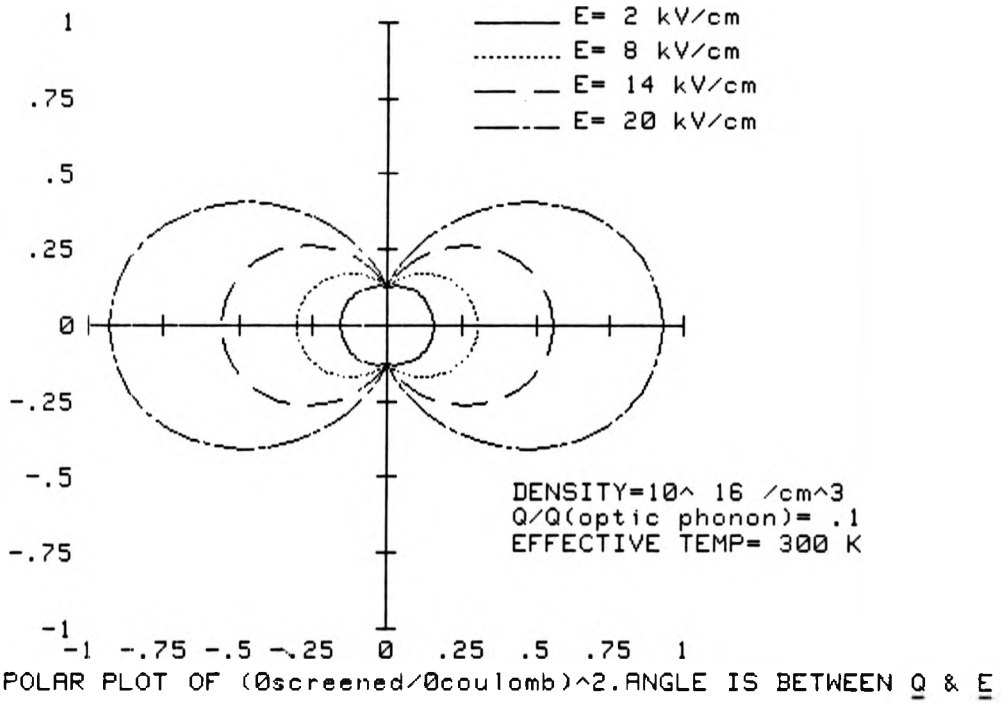

E= 2 kV/cm
E= 8 kV/cm
E= 14 kV/cm
E= 20 kV/cm
1
.75
.5
.25
0
-.25
-.5
-.75
-1
-1 -.75 -.5 -.25 0 .25 .5 .75 1
DENSITY=10^ 16 /cm^3
Q/Q(optic phonon)= .1
EFFECTIVE TEMP= 300 K
POLAR PLOT OF (0screened/0coulomb)^2.ANGLE IS BETWEEN Q & E

Fig. 5.4.12.

However what the model does not allow for is a variation in the distribution function and the inclusion of a damping effect from the energy loss due to collisions (recall the Landau damping inherent in the formalism is a collisionless energy loss mechanism).

Both of these considerations should lead to a diminishing of the field effects on the basis of intuitive arguments. Finite collisional damping will destroy the sharp δ-function form of energy conservation in the spectral function due to the randomising produced by a collision, and the consequent spread in energy will mean the field effect is averaged over this range.

Similarly if we consider a change in the distribution function, particularly one in which the peak of the distribution is shifted away from the zero momentum position (such as in displaced Maxwellian schemes popular in hot electron transport theory[71]) then since the maximum field effect occurs at zero momentum transfer the act of displacing the maximum population away from this optimum wavevector value will reduce the field effect since the peak will give a stronger weighting to less important wavevector values. It would not be unreasonable to assume a combination of these effects could wash out any significant field dependence and so we must attempt to include these effects in the model.

The effects of constant collisional damping may be involved by going back to the original form of the spectral function (4.6.29.) under the Local-Homogeneity-Approximation. The assumption used so far in this chapter is that the imaginary part of the self energy ($\Gamma(RTP\omega)$) may be considered vanishingly small so that we are treating the electrons as infinite lifetime quasi-particles with δ-function energy spectral relations. If we now assume the collisional damping may be modelled by a finite, constant electron lifetime (and so Γ is assumed independent of $(RTP\omega)$) then the spectral function is represented by the Lorentzian form

$$a(P\omega) = \frac{\Gamma}{[\omega - \varepsilon(p)]^2 + (\Gamma/2)^2} \tag{5.4.6.}$$

To model a change in the distribution function it would be convenient if we could use a displaced Maxwellian

$$f(k) = e^{-\beta[\varepsilon(k-k_d)-\xi]} \tag{5.4.7.}$$

in the calculation of the screening function, where k_d the displacing wavevector may be chosen arbitrarily. Unfortunately (5.4.7.) is too complicated an expression (even using a quadratic dispersion relation) to allow much analytic reduction of the general form (5.1.6.). However we can go some of the way if we assume that the displacing wavevector is sufficiently small to allow us a Taylor expansion of (5.4.7.) in the form

$$f(k) \equiv e^{-\beta[\varepsilon(k)-\xi]} \{1 + 2\lambda k \cdot k_d\} \tag{5.4.8.}$$

where λ has the usual meaning associated in (5.2.6.). Moreover if we take k_d parallel to q (so that $k \cdot k_d/|k_d| \equiv k \cdot q/|q|$) it is possible to use the model expressions (5.4.8.) and (5.4.6.) to derive a model screening function that includes both collisional damping and a displaced distribution function. The details are standard, if laborious, and so we only quote the result here (the details are expanded in Appendix VIII) giving the desired screening function:

$$\begin{aligned}\varepsilon[q,\omega_E,\Gamma,k_d] = &\left[1 + \frac{2\kappa_D^2 k_d}{q^3}\right] \\ &+ x\left[\frac{\kappa_D^2 k_d}{q^3}\right][Z(x - \tfrac{a}{2}) + Z(x + \tfrac{a}{2})] \\ &+ \left(\frac{\kappa_D}{q}\right)^2\left[1 - \frac{k_d a^2}{q}\right]\frac{[Z(x - \frac{a}{2}) - Z(x + \frac{a}{2})]}{2a}\end{aligned} \tag{5.4.9.}$$

where all parameters have previously been introduced and take on the same values except for the variable x which now has a finite imaginary part due to the collisional damping modifying the field induced frequency. Explicitly

it now becomes (compare with (5.2.9.))

$$x_{E,\Gamma} = \sqrt{\frac{\beta m}{2}}\sqrt{\frac{eE}{2qm}} + \frac{i\Gamma}{2}\sqrt{\frac{2m\beta}{\hbar^2 q^2}} \qquad (5.4.10.)$$

It is clear that if the displacing wavevector k_d and the damping Γ are set equal to zero, this new model screening function (5.4.9.) collapses to the previous model field dependent form (5.4.2.(a)) as of course it should.

Thus in an identical fashion to (5.4.5.) we will now consider the ratio of the screened potential shielded by (5.4.9.) to the bare Coulomb potential. The resulting plots of

$$\left|\frac{\phi_s[q,\omega_E,\Gamma,k_d]}{\phi_{Coulomb}}\right|^2 = \left|\frac{1}{(5.4.9.)}\right|^2 \qquad (5.4.11.)$$

will correspond to Figure (5.4.9.-11.) but with the inclusion of damping and displacing.

The calculations of the Plasma function involved in the subsequent graphs are performed slightly differently to the previous pictures since now, because of (5.4.10.), the phase velocity is a complex number. This means that the imaginary part of the Plasma Function is no longer a decaying exponential but is as complicated a function as the real part. Consequently the Padé approximant derived in Appendix (VI) is used to calculate both real and imaginary parts of the screening function (5.4.9.) even when the collisional damping is set equal to zero.

Using this calculational procedure if we plot (5.4.11.) for <u>zero</u> damping and displacing, the resulting picture will act as the 'standard' to which the rest should be compared. This standard is Figure (5.4.13.) shown overleaf where we take an electron concentration of 10^{16} cm^{-3} at 300 K being driven by electric fields between 2 and 20 kV cm^{-1}.

The next two Figures are plots of the same function (5.4.11.) showing the changes brought about by displacing the distribution function by one-hundredth and one-tenth of an optic phonon wavevector respectively keeping

it now becomes (compare with (5.2.9.))

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It is clear that if the displacing wavevector k_d and the damping Γ are set equal to zero, this new model screening function (5.4.9.) collapses to the previous model field dependent form (5.4.2.(a)) as of course it should.

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$$\left|\frac{\phi_s[q,\omega_E,\Gamma,k_d]}{\phi_{Coulomb}}\right|^2 = \left|\frac{1}{(5.4.9.)}\right|^2 \qquad (5.4.11.)$$

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The next two Figures are plots of the same function (5.4.11.) showing the changes brought about by displacing the distribution function by one-hundredth and one-tenth of an optic phonon wavevector respectively keeping

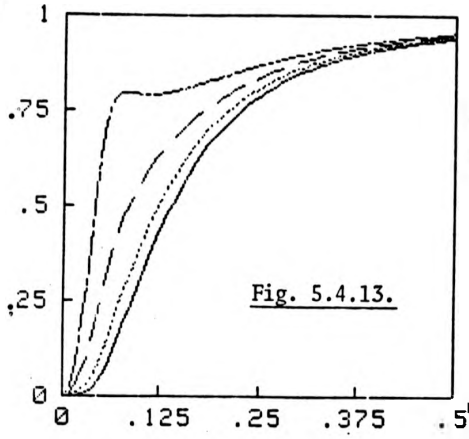


Fig. 5.4.13.

_____ E= 2 kV/cm
..... E= 8 kV/cm
— — — E= 14 kV/cm
—·—·— E= 20 kV/cm

DENSITY= 1E+16 /cm^3
EFFECTIVE TEMP= 300 K
DAMPING= 0 *OPT.PHONON ENERGY
DISPLACING WAVEVECTOR
= 0 *OPT.PHONON

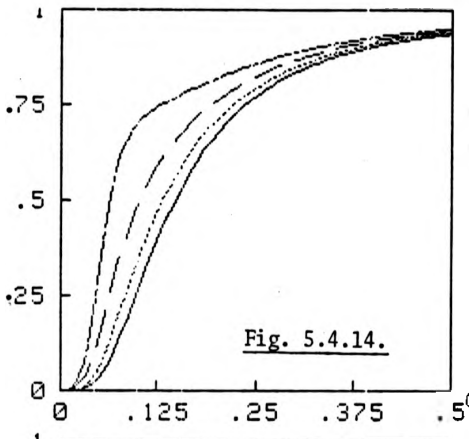


Fig. 5.4.14.

_____ E= 2 kV/cm
..... E= 8 kV/cm
— — — E= 14 kV/cm
—·—·— E= 20 kV/cm

DENSITY= 1E+16 /cm^3
EFFECTIVE TEMP= 300 K
DAMPING= 0 *OPT.PHONON ENERGY
DISPLACING WAVEVECTOR
= .01 *OPT.PHONON

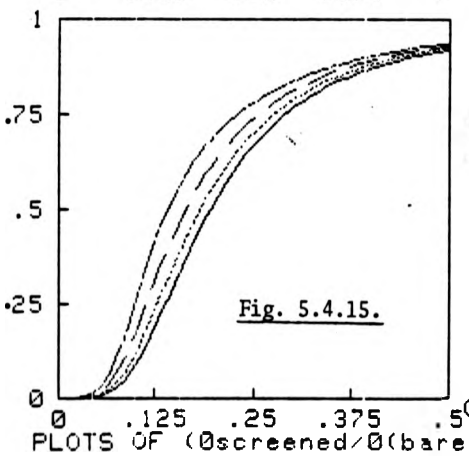


Fig. 5.4.15.

_____ E= 2 kV/cm
..... E= 8 kV/cm
— — — E= 14 kV/cm
—·—·— E= 20 kV/cm

DENSITY= 1E+16 /cm^3
EFFECTIVE TEMP= 300 K
DAMPING= 0 *OPT.PHONON ENERGY
DISPLACING WAVEVECTOR
= .1 *OPT.PHONON

PLOTS OF (0screened/0(bare Coulomb))^2.

the collisional damping zero.

They clearly exhibit the expected behaviour of reducing the interaction field effect but it remains significant still (particularly when we recall these plots are comparisons against the bare Coulomb potential).

We can now change parameters and obtain the corresponding plots of (5.4.11.) for zero displacing wavevector but with a collisional damping energy equivalent to one-hundredth and one-tenth the optic phonon energy. The respective diagrams are Figures (5.4.16.) and (5.4.17.).

Comparing these figures with (5.4.13.) it is evident that the inclusion of collisional damping does not significantly reduce the magnitudes of these curves of any particular wavevector value (in fact the opposite is true particularly at small wavevector values). The obvious peculiar effect occurs at long wavelengths where we would, as a first guess, expect all curves to tend to zero whereas in actual fact they tend to a finite value which increases as the damping increases.

It is not obvious but this is a feature of employing a constant (i.e. independent of q and E) damping rate Γ in the model screening function as may be seen by examining the $q \to 0$ limit of (5.4.11.) as follows. Since $k_d = 0$ the long wavelength limit of (5.4.9.) is just

$$\epsilon[q,\omega_E(\Gamma)] = 1 + \left[\frac{\kappa_D}{q}\right]^2 [1 + xZ(x)] \qquad (5.4.12.)$$

where, from (5.4.10.)

$$x \equiv x_{E,\Gamma} = A\sqrt{\frac{E}{q}} + \frac{iB}{2}\,\Gamma/q \qquad (5.4.13.)$$

and A,B are constants.

Hence for small q (large x) the asymptotic expansion of the Plasma Function (VI.6.) combined with (5.4.13.) when substituted into (5.4.12.) yields

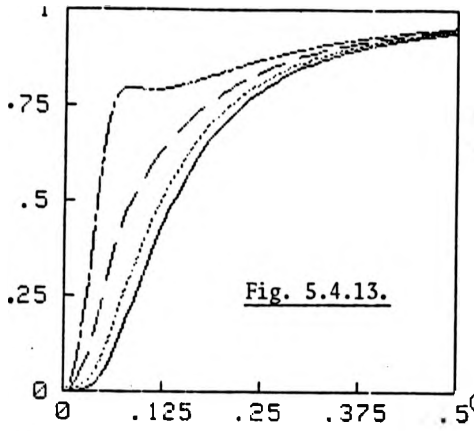


Fig. 5.4.13.

———————E= 2 kV/cm
..... E= 8 kV/cm
— — — — E= 14 kV/cm
—.—.—.—.E= 20 kV/cm

DENSITY= 1E+16 /cm^3
EFFECTIVE TEMP= 300 K
DAMPING= 0 *OPT.PHONON ENERGY
DISPLACING WAVEVECTOR
= 0 *OPT.PHONON

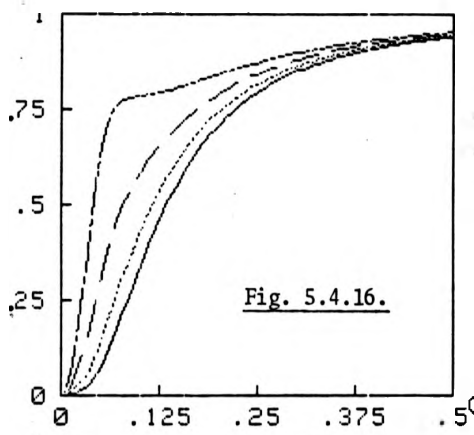


Fig. 5.4.16.

———————E= 2 kV/cm
..... E= 8 kV/cm
— — — — E= 14 kV/cm
—.—.—.—.E= 20 kV/cm

DENSITY= 1E+16 /cm^3
EFFECTIVE TEMP= 300 K
DAMPING= .01 *OPT.PHONON ENERGY
DISPLACING WAVEVECTOR
= 0 *OPT.PHONON

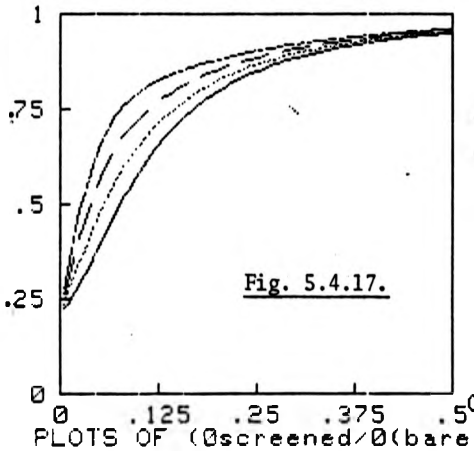


Fig. 5.4.17.

———————E= 2 kV/cm
..... E= 8 kV/cm
— — — — E= 14 kV/cm
—.—.—.—.E= 20 kV/cm

DENSITY= 1E+16 /cm^3
EFFECTIVE TEMP= 300 K
DAMPING= .1 *OPT.PHONON ENERGY
DISPLACING WAVEVECTOR
= 0 *OPT.PHONON

PLOTS OF (0screened/0(bare Coulomb))^2.

$$\epsilon[q,\omega_E] \simeq 1 - \frac{\kappa_D^2}{2}\left[\frac{A^2Eq - B^2\Gamma^2/4}{(A^2Eq - B^2\Gamma^2/4)^2 + A^2B^2\Gamma^2Eq}\right] + i\frac{\kappa_D^2}{2}\left[\frac{AB\Gamma\sqrt{Eq}}{(A^2Eq - B^2\Gamma^2/4)^2 + A^2B^2\Gamma^2Eq}\right] \qquad (5.4.14.)$$

from which it may be seen that if $\Gamma = 0$ then in the limit of $q \to 0$, $Re\epsilon = \lim[1 - \kappa_D^2/2A^2Eq]$ which diverges and $Im\epsilon \to 0$. Consequently in plots of $1/|\epsilon|^2$ the curves will always tend to zero for $\Gamma = 0$. However if $\Gamma \neq 0$ then the limiting behaviour is different since then

$$\lim_{q\to 0} Im\epsilon \propto \sqrt{q} \to 0$$

and

$$\lim_{q\to 0} Re\epsilon = 1 + 2\kappa_D^2/B^2\Gamma^2$$

which is a finite quantity and thus in Figures (5.4.16.) and (5.4.17.) the limiting behaviour will tend to $1/(1 + 2\kappa_D^2/B^2\Gamma^2)^2$ which is an increasing function of Γ bounded by 0 and 1.

To reiterate, if the effects of collisions are modelled by a constant damping rate then in plots of $1/|\epsilon|^2$ the limiting behaviour as $q \to 0$ will tend to a non-zero value somewhere between 0 and 1, as a distinction to the zero damping case where the curves will always tend to the origin.

Although this successfully explains the behaviour of Figures (5.4.16.) and (5.4.17.) it should be noted that the model used to describe collisional damping is unphysical since we would expect the damping to depend at least on the particles' energy. Estimates of collisional damping using a simple Boltzmann equation with binary collisions have given a variation of Γ that tends to zero with q (see for instance Totsuji[94]) in which case the limiting behaviour of the damped curves should be the same as the undamped ones. The correct treatment of course should utilise the imaginary part of the self energy obtained in Chapter 3, but as we have commented several times already, this would involve a very complicated self consistent calculation. In the absence of any critical calculations of the damping, the model used

here should be considered as qualitative only, but since a constant damping rate will tend to overestimate the true values the conclusions of Figures (5.4.16.) and (5.4.17.) should still hold in that even for strong collisional damping there will still remain a significant interaction-field-effect.

Thus we have now studied the sensitivity of the interaction-field-effect to temperature changes, alterations in the electron concentration, variations in the field strengths and angles they make with the momentum transfer, changes in the distribution function and finally, of the possible consequences of allowing the randomisation generated in a collision to dampen these effects. Although a comprehensive summary of the results is left to the conclusion of this chapter, at this stage it seems as if a strong electric field (kilovolts per cm) acting within a collision can significantly alter the calculated transition rates. It would appear the effects are most powerful in very high fields on low density low temperature systems where strong inhomogeneities will be apparent and may only be qualitatively altered if the distribution function and damping rates are varied.

The analysis of this section has been concerned with a three dimensional electron plasma, but there are (quasi-) two dimensional electron systems where similarly it may be possible to observe an interaction-field-effect. As a consequence of the two-dimensionality, correlation effects are more pronounced in such systems primarily due to the lack of this extra dimension into which carriers may scatter and disperse the correlations. Therefore interaction effects should be stronger in such systems and so it is to such situations we now turn our attention.

§5.5. The two-dimensional Maxwellian screening function

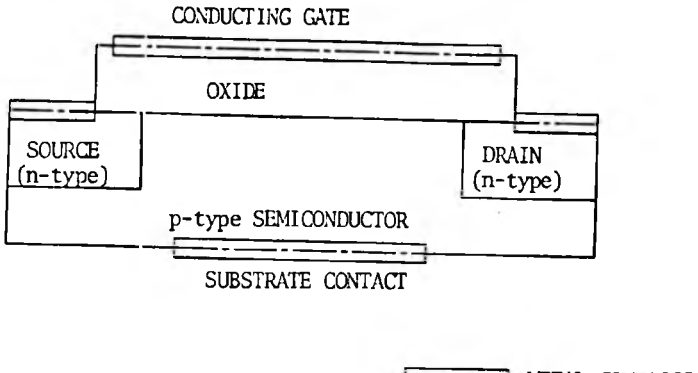
Up until now we have been examining the behaviour of an electron plasma in high electric fields in order to model various processes expected to occur in very small bulk semiconductor devices and in particular the deviations brought about because this field can act during a collision event. However

in recent years a great deal of interest has been focused on the behaviour of two-dimensional electron plasmas primarily due to the conditions created in two specific physical situations.

The first one occurs at the surface of certain bulk dielectrics such as liquid Helium or Neon at very low temperatures where bound electron surface states form a quasi-two-dimensional system parallel to the surface (the first numerical investigation of this phenomenon was undertaken by Cole and Cohen[22] and was experimentally verified by Brown and Grimes[20] in 1972). In such systems the accessible areal electron density is typically in the range of 10^5 - 10^9 electrons cm^{-2} and the corresponding Fermi temperatures between 10^{-6} and 10^{-2} K. Since the experiments are usually performed at a temperature of $\sim$ 1 K, these two-dimensional electron plasmas are expected to exhibit classical behaviour. Various discussions on the behaviour of classical 2-D plasmas exist (see for instance Fetter[31] Totsuji[94] and Studart and Hipolito[88]) however it would appear that the very low densities involved demands a more rigorous many body approach to incorporate the relevant correlations in low density systems[66].

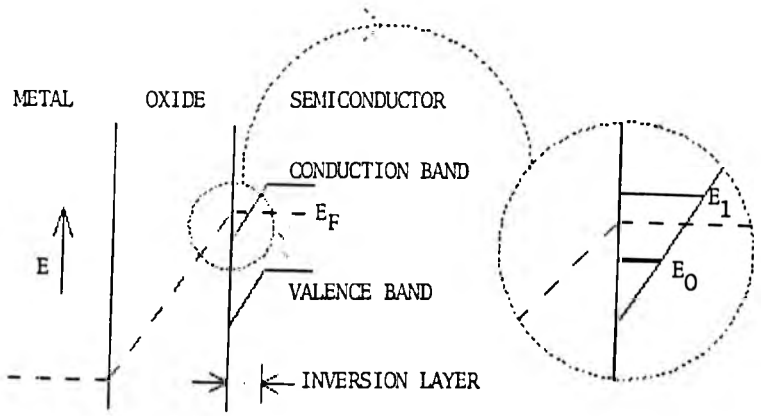
The second situation occurs at interfaces of semiconductors where quantisation in inversion layers can lead to constrained motion perpendicular to the interface thus forming a two-dimensional electron plasma. The difference between the two situations is in the experimental areal electron density since, in inversion layers, we are typically concerned with the much higher densities of 10^{11} - 10^{13} cm^{-2}[86] (a good review of semiconductor inversion layers may be found in the Proceedings of International Conferences on the electronic properties of 2-D systems I, II, III[89]).

The essential physics for the formation of these high density electron plasmas is illustrated using the following diagrams of a p-type metal-oxide-semiconductor transistor (MOSFET) as an example.



SCHEMATIC DIAGRAM OF A P-TYPE MOSFET

Fig. 5.5.1.



BAND BENDING STRUCTURE AT THE INTERFACE

Fig. 5.5.2.

Basically this device is a parallel plate capacitor with the semiconductor constituting one plate. A voltage difference across the two plates produces opposite charges on each and an electric field intensity across the interface which acts as a potential barrier. If the conducting gate is biased positively in this p-type device, the few electrons there are in the bulk congregate in a thin region close to the interface which constitutes the inversion layer allowing an electrical contact between source and drain which permits measurement of the conductivity through the channel for instance. Since the electron population in this inversion layer will depend on the (controllable) gate voltage it is possible to study many body effects due to the electron-electron interaction since the above configuration allows one to vary the electron density precisely over some three orders of magnitude in just one particular sample[84]. The controllability of the inversion layer concentration combined with the occurrence of very high electron mobilities in these devices[24] makes them technologically important physical systems.

One consequence of these strong inversion layers is that the energy bands are distorted downwards at the interface (Figure 5.5.2.) and if the inversion is strong enough the bands fall below the Fermi level producing a deep, almost triangular, potential well which forces the electrons into quantised energy levels (Figure (5.5.2.)).

Since the energy levels are split typically by about 10 meV[86] then if the effective electron scattering rate is sufficiently small (which will depend primarily on the electron density and temperature) the electrons in the lowest subband are confined to move in a quasi-two-dimensional system, needing an energy in excess of 10 meV to move perpendicular to the interface.

Although the technological impetus behind quantised inversion layers has given rise to a great deal of effort expended on the study (both theoretical and experimental) of high density two-dimensional plasmas, it is fair to say that the various theories of electronic processes in such systems (and in particular we refer to the recent works of Jonson[50] Mori

and Ando[68] and Stern[85]) can still at best only give qualitative agreement with experimental observations (Bishop et al.[15] and Störmer et al.[81]). Specifically we refer to the problems encountered with the electron mobility where calculated values[68][85] are consistently three or four times larger than what is observed[24][87] and the hitherto unexplained behaviour of the electron effective mass in magnetoconductance experiments on p-type Si MOSFETs where this effective mass increases slightly as the electron concentration drops below 10^{12} cm^{-2}[86]. It has been suspected that both of these anomalies are due to electron-electron interaction effects[92] and in particular Bishop et al.[15] make the point that discrepancies between theory and experiment are at least partly connected with our lack of understanding of the screening process.

This is an encouraging sign from the point of view of this thesis since it is precisely in these type of systems that the interaction-field-effect could make a noticeable contribution. Thus although our results are not directly transposable to these low temperature experiments we should hope that overall behaviour will lead to specific conclusions as to the deviations of electronic processes within the interaction field effect.

Therefore in order to gain some insight into the peculiarities of field dependent screening in inversion layers we will now repeat most of the calculations of the last section, but including the modifications due to the reduced dimensionality. In particular this will mean a modified density of states (which is independent of energy in two-dimensions) and two dimensional equivalents of the bare Coulomb potential $\phi_{2D}(q)$ and the inverse Debye screening length κ_{2D}.

Therefore with due account of these modifications it is a straightforward matter to obtain a two dimensional screening function using a Maxwellian distribution function. The details are reserved for Appendix (VII) and we only quote the result here. Specifically we find

$$\epsilon[q,\omega_E] = 1 + \left(\frac{\kappa_{2D}}{q}\right) \frac{[Z(x - \frac{a}{2}) - Z(x + \frac{a}{2})]}{2a} \qquad (5.5.1.)$$

where (x) and (a) are the same dimensionless variables used in the preceding section and κ_{2D} is the inverse two dimensional screening length (VII.15.). Thus we see that (5.5.1.) is obtained from its' three dimensional counterpart by the simple subsititutions of $\kappa_{3D} \to \kappa_{2D}$ and $(\kappa_{3D}/q)^2 \to (\kappa_{2D}/q)$.

Without going into details we note that (5.5.1.) may be used to study the static and dynamic behaviour of a classical two-dimensional electron plasma in a fashion analogous to §5.3. since the classical limit of (5.5.1.) is just

$$\epsilon[q,\omega_E] = 1 + \left(\frac{\kappa_{2D}}{q}\right)[1 + xZ(x)] \qquad (5.5.2.)$$

the zero field limit of which gives the conventional Debye screening in two dimensions i.e.

$$\epsilon[q] = 1 + \frac{\kappa_{2D}}{q} \qquad (5.5.3.)$$

Similarly the analysis of the potential created by a moving test charge with velocity $u = x\langle v\rangle$ may be obtained as

$$V(R) \equiv V(r - ut) = \frac{e^2}{4\pi\epsilon_\infty} \int_0^\infty dq \, \frac{qJ_0(qR)}{q + \kappa_{2D}[1 + xZ(x)]} \qquad (5.5.4.)$$

A similar expression to (5.5.4.) has been used by Studart and Hipolito[88] in their deliberations of the classical 2-D plasma where our function $1 + xZ(x)$ is referred to as a local field correction. However in the context of (5.5.4.) it is just the explicit dependence of the screening on the electrons' velocity. If $\kappa_{2D}[1 + xZ(x)] \equiv \kappa^*_{2D}$ is a positive quantity (i.e. for small test speeds) then (5.5.4.) may be expressed in terms of Struve (H_0) and Neumann (Y_0) functions[2] as

$$V(R) = \frac{e^2}{4\pi\epsilon_\infty}\left[\frac{1}{R} - \frac{\pi}{2}\kappa^*_{2D}\{H_0(\kappa^*_{2D}R) - Y_0(\kappa^*_{2D}R)\}\right] \qquad (5.5.5.)$$

The form of this potential is strikingly different to its' three dimensional counterpart (5.3.9.) as may be exhibited in its' asymptotic behaviour where for large R (5.5.5.) may be expanded as

$$V(R) \simeq \frac{e^2 \kappa^*_{2D}}{4\pi} \left[\frac{1}{(\kappa^*_{2D}R)^3} - \frac{9}{(\kappa^*_{2D}R)^5} + \frac{225}{(\kappa^*_{2D}R)^7} \ldots \right] \qquad (5.5.6.)$$

from which it is evident that this effective potential decays algebraically as opposed to exponentially. Consequently the correlations should be active over large distances in two-dimensional systems and it has been conjectured that the existence of long range correlations could induce the electron assembly to crystallise into a regular array. However there is no conclusive evidence yet as to the formation of such a Wigner lattice, and so the reality of such a crystallisation remains uncertain. It is interesting to note though that (as in the three-dimensional case) for a critical value of the test speed the effective inverse screening length will tend to zero and become negative. This will produce a divergence in the potential at long distances as can be seen in (5.5.6.) indicating an instability in the electron plasma (recall though that this makes no allowance for the imaginary part of the Plasma Function which would prevent any strict divergence). Thus we see that the formalism of the interaction field effect may be used to study the dynamic properties of the two-dimensional electron gas - an interesting and currently active subject in its' own right.

However our concern is with the field-induced variations in the squared interaction potential since this is the quantity that will directly influence the mobility of carriers, through the transition rates. Therefore as in §5.4. we consider the squared ratio of the screened to the bare Coulomb interaction in two-dimensions i.e.

$$\left|\frac{\phi_s[q,\omega_E]}{\phi_{Coulomb}}\right|^2 \equiv \left|\frac{q}{q + \kappa_{2D}[Z(x - \frac{a}{2}) - Z(x + \frac{a}{2})]/2a}\right|^2 \qquad (5.5.7.)$$

and first of all plot this function to exhibit the electron concentration dependence. Therefore for parameters appropriate to bulk GaAs at a temperature of 150 K the following two diagrams overleaf for electron areal densities of 5×10^{11} and 10^{11} cm^{-2} respectively being acted upon by electric fields in the 1 to 10 kV cm^{-1} range.

There are three obvious characteristics to these diagrams. First, if we compare these figures with their three-dimensional counterparts we note that Figures (5.5.3.) and (5.5.4.) have a much more gradual rise to the bare Coulomb value of unity. This is because the three dimensional screening function depends on $1 + 1/q^2$ as opposed to $1 + 1/q$ in this case.

Secondly the dependence on density is extremely sensitive particularly in the small q limit where it is seen that the interaction field effect has a very powerful influence and the high field values exhibit the anti-screening phenomenon (in the sense that the magnitude of the screened potential is greater than the bare Coulomb potential in a range of q-values) introduced in the previous section. However the anti-screening is achieved much more easily in this two dimensional system and can only be a consequence of correlation effects being more important in such situations. This is also why the field effect (which is undoubtedly significant in Figure (5.5.4.)) is more pronounced, as indicated by a comparison of diagrams (5.5.4.) and (5.4.9.). We note that these diagrams justify the closing comments of §5.4.

The third feature of these pictures is the resonant-like behaviour of the function as $q \to 0$ and is a peculiarity of the field effect in two dimensions (recall the 3-D case always went to zero as $q \to 0$). It may easily be explained by analytic considerations of the long wavelength screening function (5.5.2.) and the definition of the field dependent variable

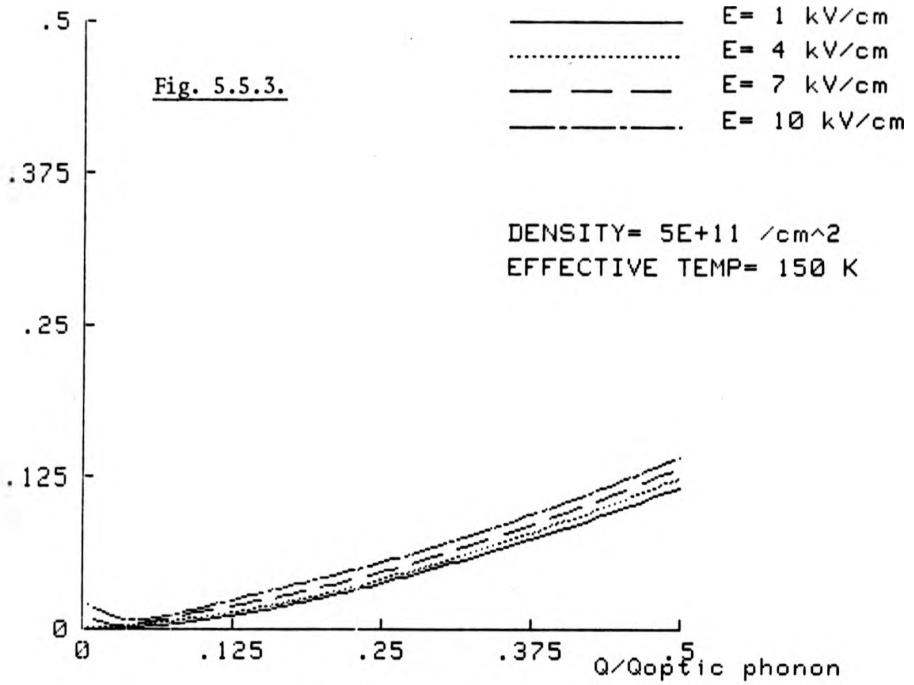


Fig. 5.5.3.

PLOT OF (Ø[screened]/Ø[bare Coulomb])^2.

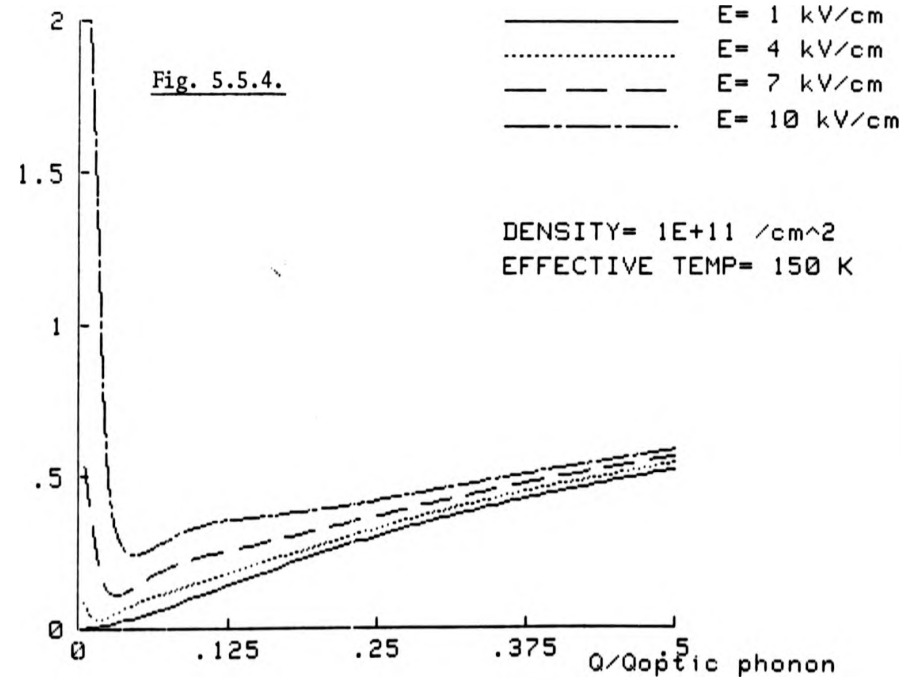


Fig. 5.5.4.

PLOT OF (Ø[screened]/Ø[bare Coulomb])^2.

$$x = \sqrt{\frac{\beta m}{2}}\frac{\omega_E}{q} = \sqrt{\frac{\beta m}{2}}\sqrt{\frac{eE}{2mq}}$$

For non zero electric fields the $q \to 0$ limit focuses attention on the large x behaviour of the Plasma Function, the imaginary part of which decays exponentially with x^2 and thus may be neglected. However using the asymptotic expansion (VI.6) gives a limiting value of the screening function of

$$\mathrm{Re}\epsilon[q \to 0, \omega_E] \simeq 1 - \frac{2\kappa_{2D}}{\beta eE} \qquad (5.5.8.)$$

which is independent of q. Therefore $1/|\epsilon|^2$ will tend to the field dependent value of $1/|1 - 2\kappa_{2d}/\beta eE|^2$ as $q \to 0$ which may take on any positive value and actually diverge for a particular choice of the electric field (which occurs at 13.7 kV cm^{-1} in this particular situation).

If we compare (5.5.8.) with the equivalent three dimensional expression

$$\mathrm{Re}\epsilon[q \to 0, \omega_E] \simeq 1 - \frac{2\kappa_{3D}^2}{\beta eEq} \qquad (5.5.9.)$$

which diverges as $q \to 0$, and hence its' inverse will tend to zero as $q \to 0$ independent of the field, we see that the behaviour of the graphs Figures (5.5.3.) and (5.5.4.) is a sole consequence of the systems two-dimensionality.

Of course the low temperature (150 K) used in these plots assisted the interaction field effect since high temperatures act to destroy correlations even in two-dimensional systems and subsequently reduce the field effect which enhances correlations.

Therefore the next two figures (5.5.5.) and (5.5.6.) illustrate how significantly a temperature change from 200 to 300 K can reduce the interaction-field-effect (all other parameters remain as in Figure (5.5.4.)). It is evident that although the effect is reduced at any particular wavevector value the field dependence is still strong and dominated essentially by the electron concentration.

If we were to look at the more realistic physical situation of doping in excess of 10^{12} electrons cm^{-2} on similar plots the effects would not be

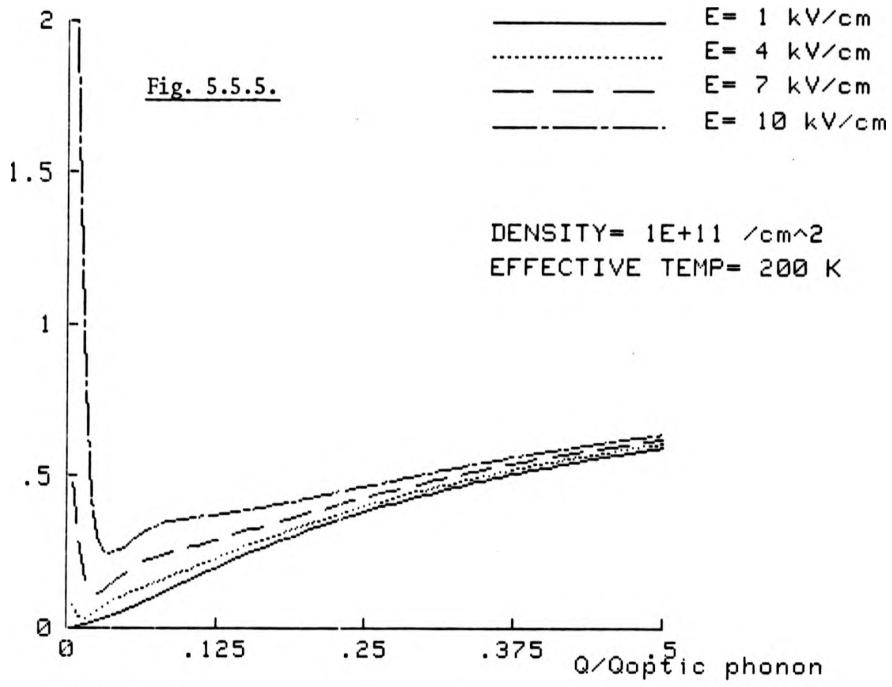


Fig. 5.5.5.

PLOT OF (Ø[screened]/Ø[bare Coulomb])^2.

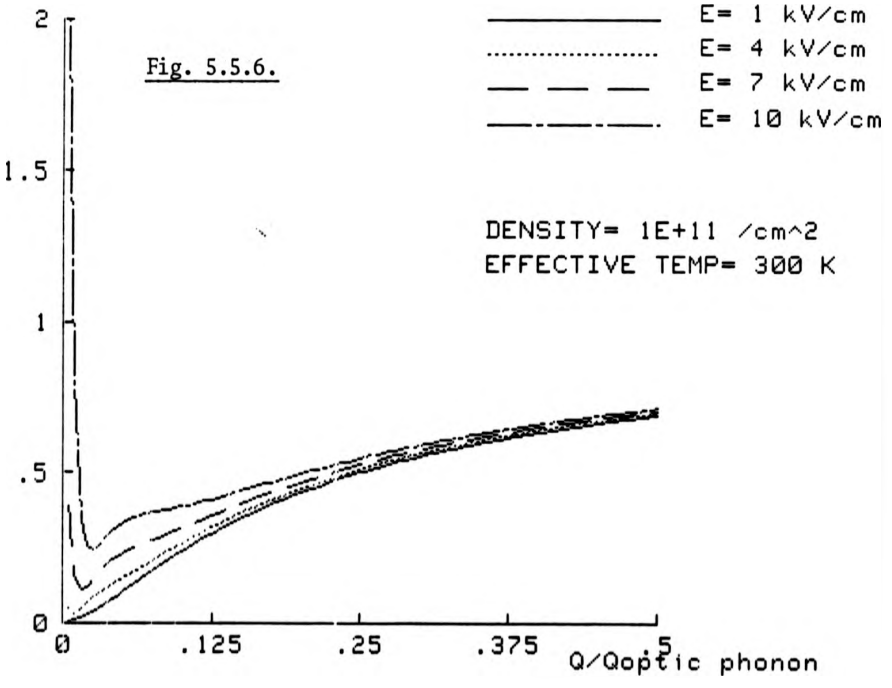


Fig. 5.5.6.

PLOT OF (Ø[screened]/Ø[bare Coulomb])^2.

so pronounced. Also since conventional calculations are performed using a Debye screening function it would seem sensible to plot the ratio of our field dependent function (5.5.1.) to the Debye form (or more rigorously the field independent form of (5.5.1.) but since this approximates the Debye form closely the ratio is almost the same). This would mean that any deviations from unity are entirely due to field effects and do not involve dependencies on screening correlations. Moreover since (5.5.9.) shows that the field dependent screening function can have a divergence in the electric field at long wavelengths we choose to plot the squared ratio of the field independent screening function to the field dependent one (which involves essentially the inverse of plots considered so far) i.e.

$$\left|\frac{\phi_s(E = 0)}{\phi_s(E)}\right|^2 = \left|\frac{q + \kappa_{2D}[Z(x - \frac{a}{2}) - Z(x + \frac{a}{2})]/2a}{q + \kappa_{2D}|Z(a/2)|/a}\right|^2 \qquad (5.5.10.)$$

It is sensible to plot this ratio since then we can anticipate the curves will generally assume values between 0 and 1. Any departure from unity indicates a field effect - if the curve is less than 1 the field dependent potential is greater than the independent case and equivalently if the curves go above unity the field dependent potential is better shielded than usual.

Thus the next plot, Figure (5.5.7.) is representative of (5.5.10.) at a temperature of 150 K and using an areal density of 10^{12} electrons cm^{-2}.

As expected even at high densities a pronounced field effect exists which substantially modifies the effective interaction obtained using a field independent screening function for all relevant momentum transfer values but especially for small q where the field dependent interaction becomes many factors greater. In effect this substantiates the conclusions of §5.4., that a conventional approach to quantum transport in general, greatly overestimates the effects of shielding a point charge particularly in strong electric fields.

Further credence is given to this belief by considerations of a field- and wavevector-dependent "screening length" which may be defined from the screening function (5.5.1.) as

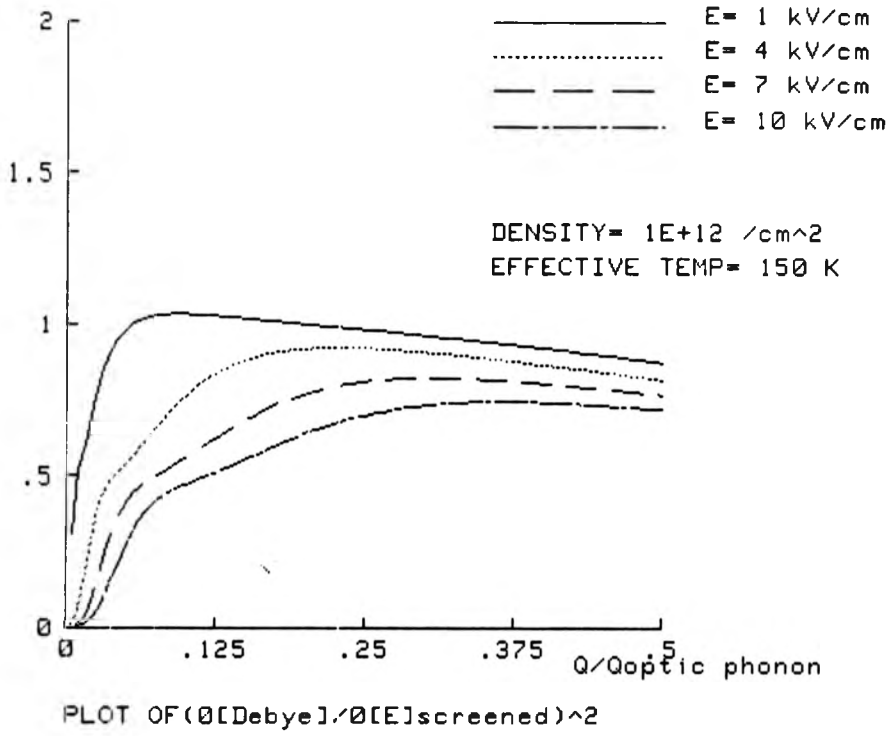

E= 1 kV/cm
E= 4 kV/cm
E= 7 kV/cm
E= 10 kV/cm
DENSITY= 1E+12 /cm^2
EFFECTIVE TEMP= 150 K
2
1.5
1
.5
0
0
.125
.25
.375
.5
Q/Qoptic phonon
PLOT OF(0[Debye]/0[E]screened)^2

Fig. 5.5.7.

$$\lambda_{2D}(q,E) = \frac{1}{\kappa_{2D}(q,E)} = \frac{1}{\kappa_{2D}} \left| \frac{2a}{Z(x - \frac{a}{2}) - Z(x + \frac{a}{2})} \right| \qquad (5.5.11.)$$

from which we obtain a q-dependent screening length $\lambda_{2D}(q)$ through

$$\frac{\lambda_{2D}}{\lambda_{2D}(q)} = \frac{1}{a} \left| \mathrm{Re} Z\left[\frac{a}{2}\right] \right| \qquad (5.5.12.)$$

which is plotted in Figure (5.5.8.).

If the Debye screening length was a good approximation the function plotted in Figure (5.5.8.) would be close to unity for all momentum transfer values. However it may only be considered reasonable in the long wavelength approximation since for large wavevector values the q-dependent screening length is much greater than the usual Debye equivalent. Since a small screening length is synonymous with efficient shielding of the potential, this diagram is further justification that 'on average' (i.e. taking into account the mean overall q-values) conventional transport allows the screening to be too efficient in reducing the range of the interactions. As a consequence of this the scattering rate taking into account field-dependent-effects will be greater than expected in conventional calculations. (Note a similar q-dependent screening length to Figure (5.5.8.) has been utilised by Stern[85] to calculate the temperature dependence of mobility in Si-inversion layers assuming a degenerate two dimensional electron system, achieving a level of qualitative comparison with experiments not possible if a constant screening length is used.)

The corresponding <u>field-dependent</u> screening lengths obtained from

$$\frac{\lambda_{2D}}{\lambda_{2D}(q,E)} = \frac{1}{2a} \left| Z(x - \frac{a}{2}) - Z(x + \frac{a}{2}) \right| \qquad (5.5.13.)$$

are depicted in Figure (5.5.9.).

The basic features are the same: the field acts to make the screening lengths even longer but now the Debye length is even a poor approximation of small q since the field effect almost destroys the screening length completely as $q \to 0$.

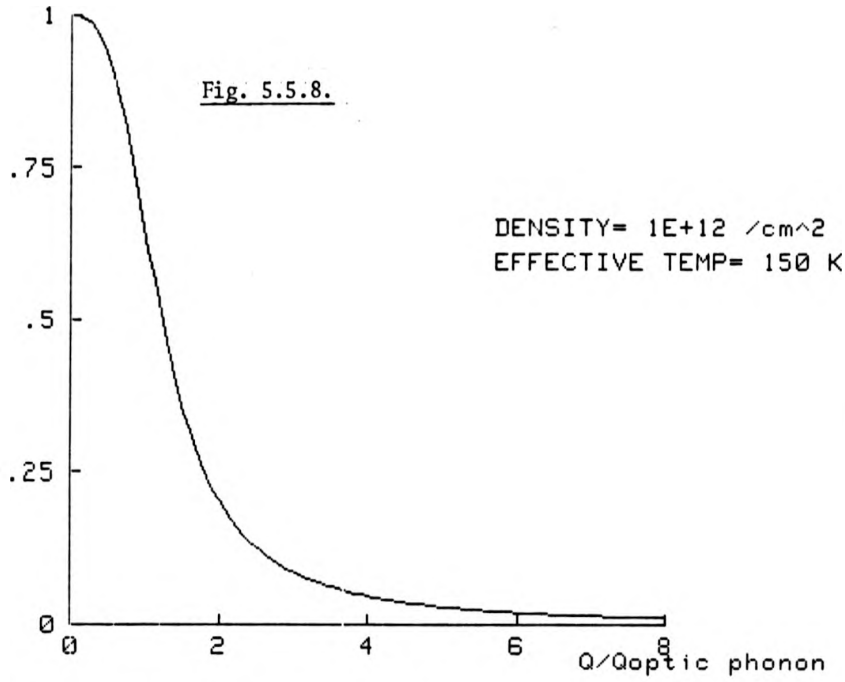


Fig. 5.5.8.

Plot of 2D Debye to q-dependent screening length

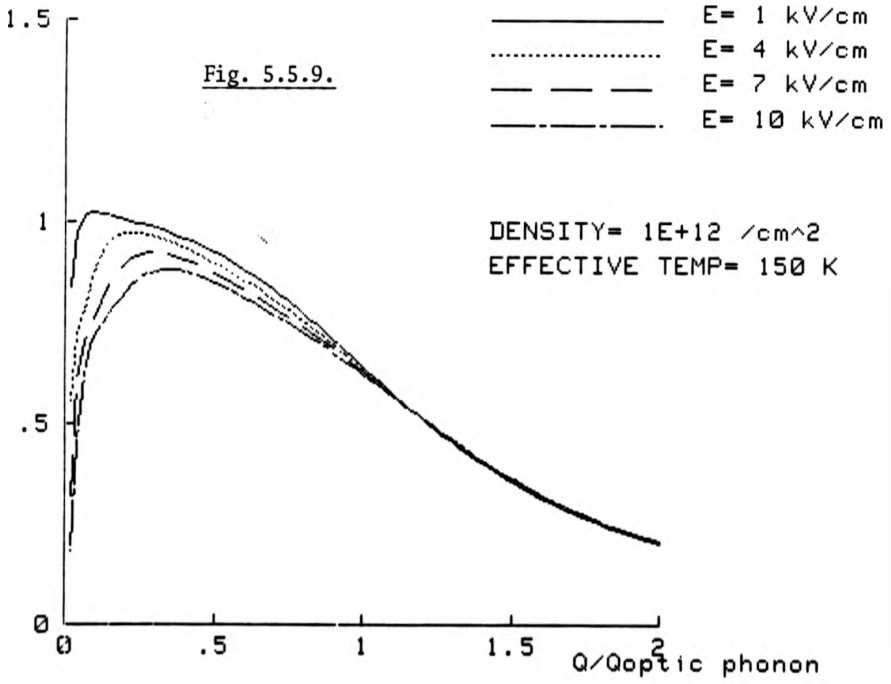


Fig. 5.5.9.

Plot of 2D Debye to field-dependent screening length

Although these figures support the notion that the interaction field effect de-screens the interaction potential it would be wise not to take these effective screening lengths too literally since (in three dimensions) the presumption might be that the potential as a function of position would decay exponentially over a range of the order of these effective screening lengths. In order for this to be a valid description though, the effective screening lengths should be independent of q at least in order to perform the inverse Fourier transform. However although their literal interpretation as screening lengths is incorrect there is no question as to the validity of them representing physical parameters which exhibit an explicit field dependence.

We have thus accomplished the aim of this section: a study of the interaction field effect on a two-dimensional Maxwellian electron plasma. Although we have briefly considered its' sensitivity to temperature fluctuations, the dominant controlling factor appears to be the electron concentration in the inversion layer which is what the pictures generally illustrated. This dependence on electron density (and by implication on the electron-electron interaction) seems to be more evident in two-dimensional systems which is almost certainly because there is a greater degree of order in such situations. Although it would be possible to obtain a screening function with scope to include collisional damping and displaced Maxwellian akin to (5.4.9.), since the studied consequences in §5.4. were slight in comparison to the density variation in three-dimensions, it seems unlikely that they will have a dominant controlling influence in inversion layer problems. Therefore this section may be considered as a supplement to §5.4. where the sensitivity of the interaction-field-effect is studied for changes in the system dimensionality. The effects encountered were generally as expected - specifically a reduced dimensionality enhances the field dependence, and the only peculiar behaviour was seen to be a consequence of working in a two-dimensional electron plasma (in particular the $q \to 0$ limit for non-zero electric fields).

We are thus in a position to synthesize the results of this chapter into a general framework which allows us to obtain a qualitative description of deviations induced by the interaction-field-effect.

§5.6. Summary

We have seen in Chapter 4 how a self consistent quantum transport theory leads quite naturally to an explicitly field dependent screening function (5.1.2.). It was noted that strong electric fields could influence the collision process in very small devices where the spatial extent of the collision becomes a significant fraction of the channel width.

In electron-electron dominated scattering a lower bound to the collision duration (5.1.9.) was estimated using the uncertainty relations from which it was possible to determine the additional energy supplied to the collision process due to the action of a constant electric field. Using this information a model screening function (5.2.12.) was obtained which was appropriate for infinite lifetime quasi-particles distributed in energy according to a Maxwellian (5.2.1.).

It was found that this screening function is controlled by the ratio of electron thermal to kinetic wavelengths and the ratio of an effective phase velocity to the thermal velocity (5.2.15.). The phase velocity derives from a field induced frequency (5.1.11.) as a direct consequence of the collisional-field-interaction which has a non zero imaginary component if the model is extended to take into account collisional damping (5.4.10.). Even in the absence of collisional damping the screening function itself has both real and imaginary components where the imaginary part may be interpreted as a consequence of Landau damping.

It was demonstrated that the classical limit of this screening function (§5.3.) reproduced the standard Debye screening theory generally considered to be appropriate for non-degenerate, high temperature plasmas. The same limit was shown to have the capability of studying the dynamic behaviour of a test charge moving uniformly through a Maxwellian plasma and the corresponding

results were in agreement with the elementary excitation approach of Pines[72].

However, of prime importance in this chapter are the modifications brought about in the squared effective interaction potential, which is a main controlling factor governing the transition rates. In order to examine any such deviations we considered first plots of the squared field independent screening potential to the Debye shielded interaction. This would make explicit the deviations introduced into the screening by the use of a q-dependent screening length. However as Figures (5.4.2.) and (5.4.3.) illustrate, the variations produced by altering the system parameters (density and temperature) are not expected to significantly alter the transition rates since the maximum difference in the squared potentials amounts to no more than 8% in the range of physically interesting parameters (although this conclusion is false if we consider an extraordinary choice of parameters such as very low temperatures and very high densities).

Having ascertained that the q-dependence of the screening length will not produce dominant effects in a submicron structure the explicit field-dependence was studied by plotting the ratio of the squared field-dependent to the independent shielded interactions (5.4.4.). The corresponding figures (5.4.4.)-(5.4.8.) clearly demonstrate that high fields produce surprisingly large deviations from conventional screening and particularly at long wavelengths. They also indicate that the effects are more pronounced for lower electron concentrations. This is because the screening is more compact for large electron densities (recall that $\lambda_D \propto 1/\sqrt{n}$) which means that the energy picked up within a collision at a fixed electric field is reduced at high densities which dampens the overall field effect.

Since the changes brought about by the field are so great when compared against the field-independent screening function, it was necessary to consider the plots of the ratio of the field-dependent effective interaction to the bare Coulomb potential (5.4.5.) since it has a better limiting behaviour in

the $q \to 0$ limit. The density dependence of this new ratio was exhibited in the sequence of figures (5.4.9.)-(5.4.11.) from which it is evident that for sufficiently high field strengths and low electron concentrations the field-dependent 'screened' interaction is actually greater than the bare Coulomb potential for a range of q-values. This is a completely unexpected result since the interpretation is that the action of a field within the collision is to de-screen the interaction and for a sufficiently strong field the interaction is actually anti-screened (i.e. the magnitude of the bare Coulomb interaction potential is enhanced).

Since this occurs at non-zero wavevector values it should not produce the unphysical scattering cross-section divergence peculiar to the Coulomb potential (since the effective potential tends to zero as $q \to 0$) but it could provide an energy loss mechanism by the excitation of plasmons. Of course such complications are completely unforseen if the transport in very small devices is modelled using conventional screening theory which, on all counts, completely overestimates the shielding efficiency and consequently underestimates the true scattering rates.

Apart from this qualitative behaviour the implications of an anti-screened interaction potential remain completely unknown at this time and obviously form a source of future work in this direction.

Having ascertained the magnitudes of this interaction-field-effect, it was exhibited in Figure (5.4.12.) how it would lead to strong inhomogeneities in direction due to the component of the electric field acting along any particular momentum transfer vector.

Just in case the effects could be considered as spurious consequences of our model screening function, the treatment was generalised to include constant collisional damping and a displaced Maxwellian distribution function into a new model screening function (5.4.9.). Although both inclusions act to reduce the interaction field effect, the resulting sequence of figures (5.4.13.)-(5.4.17.) illustrate that we still obtain significant effects even

with the inclusion of strong damping and distorted electron distribution functions.

We then commented that a reduction in the dimensionality would bring about even more pronounced field effects and consequently would be easier systems in which to spot the interaction field effect experimentally. Therefore since (quasi-) two-dimensional electron plasmas physically occur at semiconductor interfaces and on the surface of liquid He or Ne, the two dimensional screening function (5.5.2.) was analysed for a Maxwellian plasma.

The plots demonstrated a very strong electric field dependence extending over larger regions of momentum transfer when compared to equivalent three-dimensional pictures verifying the increased effect in reduced dimensions. They are similarly very sensitive to density variations and, peculiar to two dimensional systems, the limiting behaviour of the curves in the limit of $q \to 0$ does not vanish, but tends to a (possibly divergent) value depending on the electric field strength. Thus, over and above the creation of two-dimensional plasmons the almost divergent behaviour in the $q \to 0$ limit may represent an instability in the system (not related to Wigner crystallisation) which should have experimental verification.

In summary then, the interaction-field-effect is demonstrated to contribute noticeably to the transition rates thus supporting a more thorough investigation of its' consequences, and in particular with regard to the predicted anti-screening phenomenon.

CHAPTER 6

CONCLUSION

§6.1. Summary of Results

This thesis has been concerned with a phase-space approach to non-equilibrium quantum transport theory. The reasons why this particular approach was followed were introduced in Chapter 2 by considering three alternative methodologies in current popular usage which were denoted the Boltzmann equation, the wave function and the equation-of-motion techniques.

The first method using a suitable Boltzmann equation and its corresponding approximate analytic solution was an example of a phenomological approach where the various components of the transport are considered locally and compounded together in an additive fashion. This model has proven invaluable in describing most of the bulk scale behaviour of large semiconductor devices characterised by the channel length being much greater than the extent of a typical collision event. However it was pointed out that it would be naive to expect this model to hold in the medium-small device where the extent of a collision becomes comparable to the free flight between collisions since then, dynamic influences occuring within the collision (and in particular the action of a strong field) not considered within the Boltzmann scheme should alter the resulting transport.

The second technique, the wave-function approach, attempted to rectify this shortcoming by calculating a suitable transition rate from a field-dependent model Hamiltonian via the use of perturbation theory on the collisional interaction. However, in order to obtain initial value solutions to the Schrödinger equation this model Hamiltonian must be oversimplified (and so at best can only usually deal with uniform, time-dependent electric fields) and moreover an a-priori assumption must be made regarding both the strength and range of the interaction itself in order that perturbation

results for the transition rates hold. Also, as was indicated in §2.2., this approach is open to interpretational ambiguities regarding the choice of an electromagnetic gauge and even the very definition of a transition rate. On top of these difficulties, a transport equation can only be obtained by substituting the calculated transition rate for the old transition rate in a phenomenological Boltzmann equation and thus introducing an element of dynamic behaviour within the collision event.

This lack of self-consistency in the construction of a transport equation was improved by the equation-of-motion technique which relied on the neglect of high order correlation functions in order that the hierarchy of coupled density matrices equations may be reduced to a one-particle equation of motion. Unfortunately the method is only practicable if a very few number of correlations are considered and then additional assumptions of instantaneous responses and homogeneity in the system are required to decouple the resulting equations. Finally the inclusion of a strong electric field renders this technique almost useless.

Having ascertained that these three techniques were independently inadequate to do justice to the high field quantum transport problem, it was decided to use a phase-space interpretation of quantum mechanics and Greens function techniques to tackle the many-body problem.

Although the phase-space description of quantum mechanics is not unique there are universal distinctions to the classical phase-space description inherent in Boltzmann transport theory. Therefore Chapter 3 introduced the Marcinkiewicz theorem, through which it was demonstrated that a quantum phase-space distribution unlike its' classical counterpart cannot in general be real, bounded and everywhere non-negative. The particular quantum phase-space distribution to be used in Chapter 4, the Wigner distribution, was then constructed as being proportional to the Fourier transform on the off-diagonal co-ordinates of the density matrix. From this definition it is clearly real and bounded and as a consequence of the Marcinkiewicz theorem

also has to assume negative values which is exhibited for a particular example in Figure (I.1.)

Having determined that it was perfectly feasible to describe quantum mechanical behaviour in a phase-space rather than state-space, Chapter 4 then proceeded to obtain coupled equations of motion for the one-electron and one-phonon Wigner distribution functions appropriate to the medium-small device. This was accomplished by the following sequence of operations.

Starting from a realistic model Hamiltonian, the exact one electron Greens function and one-phonon correlation function were obtained in terms of electron and phonon self-energies. The self energies involving the many-body correlations were subsequently approximated using functional derivative techniques where these derivatives of the collisional self-energies were neglected. This level of approximation was denoted the nesting approximation and was diagrammatically analysed in §4.8. where it was shown to be equivalent to a decomposition of the two-electron Greens function into the direct product of two one-electron Greens functions plus a screened exchange part and was valid for high density systems. A further assumption, the local-homogeneity-approximation was introduced which allowed iterative integral expressions to be Fourier transformed into closed algebraic ones which was valid as long as the change in the collisional self energy over the extent of a collision was much less than the total self energy. This was equivalent to assuming that the whole system may be considered as macroscopic when compared to the size of a collision. It was then possible to Wigner transform the Greens function equations and use the relationships listed in Appendix I to convert Greens functions into products of Wigner distributions and spectral functions. These spectral functions were seen to be related to the steady-state spectral functions but evaluated along a classical phase-space trajectory being driven by the effective electric field.

The resulting coupled equations-of-motion for the one-electron and one-phonon Wigner distributions were reminiscent of the corresponding Boltzmann

equations and as such were amenable to a quasi-particle interpretation. The lefthand-sides were of the classically expected form where the electrons were driven by an effective driving field including the Hartree contributions from the surrounding electron and phonon densities and where the phonons moved with a renormalised group velocity due to the interaction with the electrons. However significant deviations occurred in the collision integrals on the right-hand-sides where the non-asymptotic behaviour of the transport was apparent in the convoluted time-and energy-integrations which invalidated any precise δ-function form of energy conservation. This implied that the collisions were not treated as point-like events and as a consequence of their extended nature, the collision integrals became explicitly field-dependent through the spectral functions. This field-dependence was manifest in two forms: first it distorted the energy conservation factors and secondly it modified the effective interactions by making the non-equilibrium dynamical screening function explicitly field-dependent.

Chapter 5 then considered the consequences of this interaction-field-effect by an analysis of various model screening functions using a Maxwellian distribution function and a constant electric field. The models allowed the Maxwellian to be slightly displaced and permitted the inclusion of constant collisional damping.

It was found that the overall effect of a strong electric field was to de-screen the interactions in the sense that the particles collided by a potential more approaching a Coulomb potential than a Debye screened one. Indeed for sufficiently, and not unreasonably, high fields the interaction was anti-screened for a range of wavevector values.

It was seen that the de-screening behaviour was strongly affected by altering the electron density being more pronounced in low temperature and low density systems where they had a reduced efficiency of completely screening a point charge.

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damping (and thus a smearing of the sharp energy conservation factors) and more significantly reduced by using a distribution function that peaked away from the zero momentum transfer value. It was also illustrated that the interaction-field-effect leads to a marked inhomogeneity in the scattering distribution at a particular momentum transfer compared to the direction of the electric field.

The effect of a constant field within an effective interaction was then considered for a two-dimensional electron plasma where it was found that the descreening and anti-screening were even more pronounced due to the ease of which locally restraining correlations may be destroyed in two-dimensions. Again the effects were exaggerated for lower electron temperatures and densities.

The general conclusion drawn from these interaction-field-effect models is that conventional transport calculations utilising Debye-screened Coulomb potentials greatly overestimate the ability of the surrounding electron density in the medium-small-device to adequately shield a test charge, particularly in the direction of the electric field and that the errors will be more apparent in lower density, temperature and dimensional systems.

§6.2. Extension of the formalism to describe quantum ballistic transport

The approximations used in Chapter 4 essentially restrict the resulting transport equations to the medium-small-device where one is allowed to make a spatial decomposition where the mean extent of a collision is of order of the mean free path between collisions but where the size of a device is still macroscopic when compared to a collision. This means that boundary influences are relatively unimportant to the resulting dynamics which are actually determined by the many-body effects of the effective driving field and the collisions.

However it is possible to extend the formalism so that it is capable of describing the very-small-device where the active channel region becomes

comparable to the mean extent of a collision. In this situation the boundary potentials control the behaviour and one may assume ballistic transport by neglecting the many body effects of collisions. This does not imply though that the Vlasov equation may be used to describe this type of transport because the local-homogeneity-approximation no longer applies. Instead the electron driving term and the phonon diffusion term must be considered in their exact non-local form derived in Appendix IV which, when coupled with the collisionless electron and phonon equations of motion, (4.3.26.) and (4.4.14.), gives respectively:

$$\left[\partial_T + \frac{P}{m}\cdot\partial_R\right] f(R,P,T) - \frac{1}{(\pi\hbar)^3}\int d^3r'd^3k' F(R + r',T)\,ci\left(\frac{2k'\cdot r'}{\hbar}\right) \frac{\partial f}{\partial k'}(P + k',R,T) = 0 \qquad (6.2.1.)$$

and

$$\partial_T\, n(R,K,T) - \frac{1}{(\pi\hbar)^3}\int d^3r'd^3k' \bar{v}(K + k',T)\,ci\left(\frac{2k'\cdot r'}{\hbar}\right) \frac{\partial n}{\partial r'}(K,R + r',T) = 0 \qquad (6.2.2.)$$

where

$$F(R + r',T) = \frac{-\partial V_{eff}}{\partial r'}(R + r',T) \qquad (6.2.3.)$$

is the effective electron driving field and

$$\bar{v}(K + k',T) = \frac{\Omega_{K+k'}}{\omega_K}\,\partial_{k'}\Omega_{K+k'} \qquad (6.2.4.)$$

is the renormalised group velocity (since we recall that Ω_K is the bare phonon frequency and ω_K is a renormalised frequency including contributions from the real part of the phonon self-energy (4.6.20)).

These quantum ballistic transport equations will only reduce to the corresponding collisionless Boltzmann equations under either one of two conditions. The first of these, as we would expect, is the semiclassical ($\hbar \to 0$) limit since the non-local driving term for instance may be expressed

as:

$$\lim_{\hbar\to 0} \frac{-1}{\pi^3} \int d^3r'd^3k'F(R + r',T)ci[2k'\cdot r'] \frac{\partial f}{\partial k'^r} (P + \hbar k',R,T) \qquad (6.2.5.)$$

$$= \frac{-1}{\pi^3} \frac{\partial f}{\partial P} (P,R,T) \int d^3r'F(R + r',T) \int d^3k'ci[2k'\cdot r']$$

which upon using the identity (IV.9.), i.e.

$$\int_{-\infty}^{\infty} dxci[\alpha x] = -2\pi\delta(\alpha)$$

reduces to the conventional classical form

$$F(R,T) \frac{\partial f}{\partial P} (P,R,T) \qquad (6.2.6.)$$

There is also another condition not related to the vanishing of $\hbar$ which allows a reduction of the quantum structure (6.2.5.) to its' local form (6.2.6.) which is that the driving field be no more than linear in position (or alternatively if the potential is constant, linear or quadratic). This follows since if we take

$$F(R + r',T) = a + b(R + r') \quad \text{with a,b constant}$$

then we may take advantage of (IV.9.) and the condition

$$\int_{-\infty}^{\infty} dx\ x\ ci[\alpha x] = 0$$

(since the cosine integral function is even) to obtain the classical form. Explicitly

$$\frac{-1}{\pi^3} \int d^3r'd^3k'(a + bR)ci[2k'r'] \frac{\partial f}{\partial k'^r} (P + \hbar k',R,T)$$

$$- \frac{1}{\pi^3} \int d^3r'd^3k'br'ci[2k'r'] \frac{\partial f}{\partial k'^r} (P + \hbar k',R,T)$$

$$= (a + bR) \int d^3k'\delta(k') \frac{\partial f}{\partial k'^r} (P + \hbar k',R,T)$$

$$= F(R) \frac{\partial f}{\partial P} (P,R,T) \quad \text{with } F(R) \equiv a + bR.$$

Similar arguments apply to the non-local phonon diffusion term except

that this second condition demands that the effective phonon group velocity be either constant or linearly varying with its' wavevector.

In terms of the dynamic evolution of an initial electron ensemble, the implications are that for interactions with a quadratic potential, the motion proceeds classically: no additional quantum structure to the initial distribution is generated due to its' interactions with such a potential.

It is interesting to speculate that this requirement of dynamic quantum effects being generated only by a coupling to higher levels of moments than the second order is related to the Marcinkiewicz theorem of Chapter 3, which similarly implied that the distribution function would evolve classically if its' moment generating function was an exponential of a quadratic polynomial only.

Of course we also recognise that the real $\frac{p}{m}\cdot\partial f/\partial r$ structure in (6.2.1.) occurs precisely because the energy-momentum relationship in the original Hamiltonian (4.1.1.) was quadratic. Had we assumed a higher order dispersion, or indeed assumed a position dependent effective mass m(R) (if we wished to model transport across an interface) so that the kinetic energy operator was

$$\hat{\varepsilon} = \hat{p}\,\frac{1}{m(R)}\,\hat{p}$$

then the electron diffusion term would similarly have involved a complicated non-local integral structure[21] convolved with the cosine integral function.

Thus we recognise that as well as describing the collision dominated regime of the medium-small-device, the Wigner distribution phase-space approach to quantum mechanics is easily extendible to describe the fully quantum ballistic transport in the very-small-device. Moreover with adequate allowances for the non-locality provided by moments higher than second order, the formalism should be able to describe the dynamic behaviour across interfaces with an arbitrary potential barrier (including surface roughness) along with the explicit quantum occurrences of device-device coupling and switching effects due to the tunnelling phenomenon.

§6.3. Experimental verifications of the interaction-field-effect

It has previously been mentioned that the transport theory developed in this thesis has been designed for a projected need when the characteristic device sizes fall in the range of 2500-250 Å and consequently there are no experiments available at present to directly test the corrections proposed here. However in this section we mention a few physical situations of contemporary interest where careful theoretical studies using Boltzmann-type transport equations have proven incapable of quantitavely reproducing the experimental results although the qualitative behaviour is essentially correct.

In particular we refer to the two-dimensional electron gas formed in inversion layers where it has been demonstrated[84] that the electron population may be continuously controlled and varied through a range of densities in the same sample. This reproducibility of various electron densities in a system where all other parameters are unaltered allows effects to be studied which must be interpreted as being due to the many-body interactions. The two quantities which have allowed the most direct interpretation of such interactions are the measurements of the electrons' effective mass[84][86] and the Hall mobility[15][24][87] (or alternatively the mean scattering rate).

The effective mass is often obtained indirectly by oscillatory magnetoconductance experiments where the amplitude A of the magnetoconductance oscillations as a function of the magnetic field (Shubnikov-de Haas oscillations) depends on the electron effective mass m* through[58]

$$A \propto \frac{(m^*/\beta H)}{\sinh\left(\frac{2\pi^2 c\, m^*}{\hbar e\, \beta H}\right)}$$

For example Smith and Stiles[84] and Stiles[86] have studied n-type (100)Si inversion layers between 1 and 2.5 K for magnetic fields of 15.6 and 29.9 kOe in the electron planar density range of 1 to 4 x 10^{12} cm^{-2}. They

found that the effective mass had a weak but significant variation with respect to the electron density in that the effective mass increased by about 5% as the density decreased from 3×10^{12} cm^{-2} to 10^{12} cm^{-2}.

This is in the opposite direction to what we would expect from non-parabolicity effects which would predict an increase in mass for an increase in electron density. Thus these experimental results are surprising and so it has been suggested[29][92] that this phenomenon is a consequence of electron correlation effects.

Unfortunately the effective mass problem is an extremely difficult calculation to attempt, depending on the full many-body interactions although the quasi-particle description proposed in this thesis supports the notion of electron correlation effects being responsible for this anomaly as follows.

We have seen in Chapter 4 that the local-homogeneity-approximation led to a spectral function of the form (4.6.29.)

$$a(R,T,P,\omega) = \frac{\Gamma(R,P,\omega)}{[\omega - \bar{\varepsilon}(R,P,\omega)]^2 + \left(\frac{\Gamma(RP\omega)}{2}\right)^2}$$

which had a spread due to the imaginary part of the electron self energy (Γ) and which peaked at a quasi-particle energy $\omega = \bar{\varepsilon}(RP\omega)$ where $\bar{\varepsilon}$ differed from the interactionless electron energy $\varepsilon(P) = P^2/2m$ by the addition of the real part of the self energy (4.6.6.)

$$Re\Sigma = P \int \frac{d\omega'}{2\pi} \frac{\Sigma^{>}(\omega p) + \Sigma^{<}(\omega')}{\omega - \omega'}$$

Thus if we assume the effective energy to have a quadratic relationship to the momentum, then the interaction effective mass m^*_{e-e} is the inverse proportionality constant, i.e.

$$\omega = P^2/2m^*_{e-e} \qquad (6.3.1.)$$

and consequently

$$\frac{m}{m^*} = \frac{\partial\omega/\partial P}{\partial\varepsilon/\partial P} \tag{6.3.2.}$$

Therefore from the consistent relationship for the renormalised energy i.e.

$$\omega = \varepsilon(P) + \mathrm{Re}\Sigma(P,\omega) \tag{6.3.3.}$$

we may isolate an interaction effective mass expression in terms of the real part of the self energy by differentiating (6.3.3.) with respect to P and using (6.3.2.). Thus from (6.3.3.)

$$\frac{\partial\omega}{\partial P} = \frac{\partial\varepsilon}{\partial P} + \frac{\partial}{\partial\varepsilon}\mathrm{Re}\Sigma(P,\omega)\,\frac{\partial\varepsilon}{\partial P} + \frac{\partial}{\partial\omega}\mathrm{Re}\Sigma(P,\omega)\,\frac{\partial\omega}{\partial P}$$

or

$$\frac{m}{m^*_{e\text{-}e}} = \frac{\partial\omega/\partial P}{\partial\varepsilon/\partial P} = \frac{[1 + \frac{\partial}{\partial\varepsilon(P)}\mathrm{Re}\Sigma(P,\varepsilon(P) + \mathrm{Re}\Sigma)]}{[1 - \frac{\partial}{\partial\omega}\mathrm{Re}\Sigma(P,\omega)]} \tag{6.3.4.}$$

Consequently we recognise from (6.3.4.) that the interaction-effective-mass depends in a complicated manner on the many body interactions through the real part of the self energy which, under the approximations used in Chapter 4 is governed by the squared effective interaction potential as may be seen by using the explicit expressions (4.6.5.), (4.7.11.), (4.7.26.) to give

$$\frac{\partial}{\partial\omega}\mathrm{Re}\Sigma(p,\omega) = -P\int \frac{d\omega'}{2\pi}\frac{d\omega''}{2\pi}\frac{d\omega'''}{2\pi}\,dP'dP''\,\frac{|\phi_s(P',\omega'')|^2}{[\omega - \omega']^2}$$

$$x\ \{a(P - P',\omega' - \omega'')a(P' + P'',\omega'' + \omega''')a(P'',\omega''')\}$$

$$x\ \{f(P'')[1 - f(P' + P'')][1 - f(P - P')] - \tag{6.3.5.}$$
$$- [1 - f(P'')]f(P' + P'')f(P - P')\}$$

Thus apart from being controlled by the electron occupancy and the spectral functions, the electron effective mass depends critically on the effective interaction potential which as we have seen in Chapter 5 depends sensitively on the strong electric field and the electron density. Consequently for $f(P) \sim 1$ then $\partial_\omega \mathrm{Re}\Sigma(P,\omega)$ is negative and so (6.3.4.) predicts the interaction effective mass is greater than in the absence of

interactions and moreover from the plots of Chapter 5 it should increase as the density decreases as is observed.

Clearly a precise calculation of this complicated problem would be desirable but it would certainly appear that if the effective mass anomaly is to be explained by electron correlation effects then due allowances ought to be made for the reduced screening efficiency of the interactions brought about by the (necessarily strong) electric fields.

The second outstanding feature between theory and experiment in two dimensional electron assemblies is the Hall mobility: the experiments of Dingle et al.[24] and Störmer et al.[87] on modulation doped GaAlAs - GaAs heterojunction interfaces yield low temperature (4.2 K) mobilities consistently three times smaller than the most careful calculations yet performed by Mori and Ando[68] using the Boltzmann equation. Also observations of the low temperature Hall resistivity in (111)-Si inversion layers led Bishop et al.[15] to concur with the screened Coulomb interaction theory as the principle scattering mechanism except that the prediction should only have been valid for weak screening (long screening lengths) yet the experiments were estimated to have been performed in dense electron systems where the screening should have been very efficient. Their only explanation was that we simply do not understand the screening process in such systems and thus the model used in calculations was probably inappropriate to describe the dynamics. Stern[85] has attempted a generalisation of the calculated scattering rates by incorporating the full wavevector and temperature dependent screening parameter in the Thomas-Fermi model to account for an increase in the scattering rate due to the wavevector dependence reducing the screening efficiency at large wavevector values (compare figures (5.5.8.) and (5.5.9.)) in low temperature (001)-Si. However the magnitude of the change is not sufficient to account for the observed difference of a factor of three in GaAs structures and so it would appear that other mechanisms are in force that reduce the screening efficiency.

However this is precisely the type of behaviour predicted by the interaction field effect as may be seen from the figures of the preceding chapter - the action of a field within a collision event destroys the Debye screened form of the interaction which tends more to bare Coulomb behaviour. The quantity of interest is of course $1/|\varepsilon|^2$ which was previously plotted for a range of electric field strengths and electron densities where it was seen that a significant reduction in the screening efficiency was produced in two-dimensional plasmas thus leading to an increased scattering rate and a reduced mobility which may help to account for the observed discrepancy.

Of course the results of Chapter 5 are not directly transposable to this situation since most experiments are performed at liquid helium temperatures and the Maxwellian assumption on the electron distribution function is a non-degenerate approximation. Obviously a repeat of the calculations of Chapter 5 but utilising a Fermi-Dirac distribution would be advantageous.

Thus we see that even though the transport theory developed in Chapter 4 has no direct experimental verifications yet, there are aspects in its' construction (notably the intra-collisional-field-effect) beyond the scope of the traditional Boltzmann equation that may help in resolving apparent anomalies in specially constructed contemporary physical systems such as the two dimensional electron gas in inversion layers. The explicit calculations of the quantitative modifications we would expect, initially from the intra-collisional-field-effect, are part of the future areas of research suggested in the final section.

§6.4. Suggested future areas of research

This concluding section outlines various aspects of this thesis that show promise as projects of future areas of research which are best pinpointed by scanning backwards through the chapters.

The immediately preceding section indicated how modifications connected with the interaction-field-effect could qualitatively modify effective mass and Hall mobility calculations by a mechanism beyond the scope of the traditional Boltzmann-Bloch approach. Thus a prime candidate for immediate consideration is the numerical calculation of such quantities using a model based on the field-dependent screening function to give quantitative support to the predicted modifications in small devices. Such calculations could then form the basis of a quasi-particle explanation of the transport in medium-small-devices since for example the polaron mobility parallel and near to interfaces should be inhomogeneously affected by the different electron-phonon coupling constants in the two adjacent media. The problem is complicated because the actual driving field is not the externally applied field but ought to be obtained consistently from Poissons equation. This suggests a second area of research where the dynamic screening of an electron should be affected as it is injected across an interface through a changing profile and hence electric field. Thus one ought to be able to calculate the transition of an electron as it changes from one quasi-particle state to another in the different media because of the changing screening function.

It may even be possible to extend such model calculations to take into account the further modifications to the scattering rates proposed in Chapter 4 such as the field-dependent spectral functions and non-locality.

The next project for future development is the analytic and numerical study of the quantum ballistic transport equations proposed in §6.2. In many respects this is the most promising immediate area of research because it neglects many of the complications arising from many body collisions and has a Vlasov equation-like structure with a non-local driving field. Thus its' solution should contrast well with the classical forms of the collisionless Boltzmann equation and since the Wigner function equations are exact and equivalent to Schrödingers equation for the wavefunction with a Hamiltonian $H = P^2/2m + V$, the accuracy of numerical solutions to these

latter two equations may be compared for consistency since they provide alternative approaches to the same problem. The difficulty associated with the numerical solution of the quantum ballistic transport equation is that the non-local driving term involves a double integral over the cosine integral function which as may be seen from figure (IV.1.) is an oscillating, though slowly decaying function of its' argument. This implies that a direct numerical solution of the equation would be lengthy and inefficient. Hopefully analytic considerations of the equation may suggest numerical algorithms to make the calculations shorter.

Apart from such calculational aspects there are various improvements that could be made to the basic theory of Chapter 4.

Firstly we recognise that the eventual transport equations were derived essentially under two assumptions. The first of these was the nesting approximation which restricted the many body correlations to high density systems. Obviously it would be physically interesting to attempt a consistent approximation scheme which is also valid for low density systems although this would not seem to be particularly relevant to the small scale devices considered in this thesis. The second and by far the most restrictive assumption was the local-homogeneity approximation which led to the semiclassical form of the resulting equations. Although a justification was given at the time that this limited the transport to the medium small device, it should be noted that without the local-homogeneity-approximation the various consistent iterative expressions could not have been isolated into algebraic forms. Thus it would be very desirable to relax the local-homogeneity-approximation in favour of a less restrictive condition such as a W.K.B. approximation for example.

It would also be desirable to extend the basic model itself by allowing for an electron-polar phonon interaction and the application of an external magnetic field in the initial Hamiltonian (4.1.1.). Neither of these extensions would be trivial. In particular since the electron-

electron and electron-polar phonon interactions both proceed via a Coulomb interaction, the functional derivative techniques would not be able to discriminate and hence separate the two electron Greens function and the mixed electron-polar phonon Greens function, a consequence of which would mean that the screening function is determined by an electron-polar phonon contribution as well as the electron polarisability.

Finally we mention that there is still much fundamental work to be performed in using the Wigner distribution as a phase-space description of quantum mechanics. It has already been mentioned that the Wigner distribution is not unique as a quantum phase space density and it may prove to be more convenient to work with a different representation (for instance a non-negative distribution or a weighted sum of Wigner distributions). Also at the moment the Wigner function approach still relies on wavefunctions for its' definition and thus it would be convenient to obtain a consistent phase-space description formalism. This would mean in addition to the dynamic problem considered in this thesis, a consideration of the equivalent eigenvalue problem allowing, for example, a decomposition of a given Wigner distribution into a complete set of stationary-state Wigner distributions satisfying the equivalent eigenvalue equations.

In conclusion then, we recognise that this thesis only scratches the surface of a very powerful formalism of quantum mechanics where much work has yet to be performed from both the analytic and numerical points of view.

APPENDIX I

PROPERTIES OF THE WIGNER DISTRIBUTION FUNCTION AND THE WIGNER EQUIVALENT OF OPERATORS

This appendix sets out the various definitions and properties used in this thesis of the Wigner phase-space distribution function and the corresponding phase-space functions representing quantum mechanical observables. A more thorough discussion regarding the general historical development of the use of Wigner functions in quantum mechanics may be found in references[4][38][45][51][69][97].

As mentioned in Chapter 3 the construction of a quantum phase-space distribution function is not unique and the terminology of a Wigner function is sometimes used to refer to any quantum distribution function[47]. However in this thesis the terminology is specifically reserved to describe the distribution function first introduced by Eugene Wigner in 1932[97] which was initially defined for the pure state wavefunction in the position representation as a distribution of the phase space of canonical co-ordinates Q and momenta P as

$$F_W(P,Q,t) = \frac{1}{(2\pi\hbar)^N}\int d\xi e^{-iP\cdot\xi/\hbar}\psi^*(Q+\tfrac{\xi}{2},t)\psi(Q-\tfrac{\xi}{2},t) \qquad (I.1.)$$

Definition (I.1.) is immediately generalisable to the case of a mixed quantum system being in one of the pure states ψ_n with a probability P_n as

$$F_W(PQt) = \frac{1}{(2\pi\hbar)^N}\int d\xi e^{-iP\cdot\xi/\hbar}\sum_n P_n\langle Q+\tfrac{\xi}{2}|\psi_n\rangle\langle\psi_n|Q-\tfrac{\xi}{2}\rangle \qquad (I.2.)$$

where it may be seen that the Wigner distribution is a partial Fourier transform on the off diagonal matrix elements of the density matrix $\hat{\rho} = \sum_n P_n|\psi\rangle\langle\psi|$.

Of course we could have equally well started off by defining the wavefunctions in the momentum representation which would have led to a Wigner

distribution of the form

$$F_W(P,Q,t) = \frac{1}{(2\pi\hbar)^N}\int d\eta e^{iQ\cdot\eta/\hbar}\sum_n P_n\langle P+\frac{\eta}{2}|\psi_n\rangle\langle\psi_n|P-\frac{\eta}{2}\rangle \qquad (I.3.)$$

The two alternative definitions (I.2.) and (I.3.) are equivalent but the symmetry between P and Q is not manifest in these expressions. However we may observe this explicit symmetry by refering back to the general definition of a quantum distribution function given in (§3.3.2.) i.e.

$$f(PQt) = \frac{1}{(2\pi\hbar)^{2N}}\int d\xi d\eta e^{-i\xi\cdot P/\hbar - i\eta\cdot Q/\hbar} \times \sum_n P_n\langle\psi_n|e^{i\xi\hat{P}/\hbar+i\eta\hat{Q}/\hbar}|\psi_n\rangle \qquad (I.4.)$$

which reduces to either (I.2.) or (I.3.) by using the commutation relations between $\hat{P}$ and $\hat{Q}$ as demonstrated in §3.3. for the case of (I.2.)

It is immediately verified from (I.2.) or (I.3.) that the projections of the Wigner distribution give the usual momentum and position probability distributions, i.e.

$$\int dQF_W(P,Q,t) = \begin{cases} |\psi(P)|^2 \text{ for a pure state} \\ \sum_n P_n|\psi_n(P)|^2 \text{ for a mixed state} \end{cases} \qquad (I.5.)$$

and

$$\int dPF_W(PQt) = \begin{cases} |\psi(Q)|^2 \text{ for a pure state} \\ \sum_n P_n|\psi_n(Q)|^2 \text{ for a mixed state} \end{cases} \qquad (I.6.)$$

and since the probability is normalised to unity we have

$$\int dPdQF_W(P,Q,t) = 1 \qquad (I.7.)$$

We can also see that the Wigner distribution is a real valued quantity by taking the complex conjugate of either (I.2.) or (I.3.). Consequently by the implications of the Marcinkiewicz theorem discussed in §3.2. since the Wigner distribution is both real and bounded then it will in general assume negative values. This is borne out in the explicit example of the Wigner distribution for the harmonic oscillator for which the wave function is

given by

$$\psi(x,n) = (m\omega/\hbar)^{1/4}(2^n n!\sqrt{\pi})^{-\frac{1}{2}}$$

$$x\ h_n\left(\frac{m\omega x}{\hbar}\right)\exp[-m\omega x^2/2\hbar]$$

and in which case the corresponding explicit Wigner function is of the form

$$F_W(PQ) = \frac{(-1)^n}{n\pi}\exp[-2H_W(PQ)/\hbar\omega]L_n^{(0)}(4H_W(P,Q)/\hbar\omega)$$

where $L_n^{(0)}$ is a Laguerre polynomial[2], h_n are hermite polynomials and $H_W(P,Q)$ is the phase space function corresponding to the Hamiltonian $H = P^2/2m + m\omega^2q^2/2$.

Although the Wigner distribution of the ground state (n = 0) of the harmonic oscillator is always positive, it is clearly seen in figures (I.1.) and (I.2.) that the second and first excited states have Wigner distributions which assume negative values (I am indebted to Dr. Barker for allowing me to use these figures).

Properties (I.5.)-(I.7.) are sum rules that any Wigner distribution must satisfy. An additional sum rule which must be obeyed is that the values of the Wigner distribution must be bounded by $(1/\pi\hbar)^N$[4].

This may be seen as follows. From definition (I.1.) we have

$$|F(PQ)|^2 = \left(\frac{1}{\pi\hbar}\right)^{2N}\left[\int d\xi e^{-2i\xi\cdot P/\hbar}\psi^*(Q+\xi)\psi(Q-\xi)\right]^2$$

$$\leq \left(\frac{1}{\pi\hbar}\right)^{2N}\int d\xi\left|e^{-2i\xi\cdot P/\hbar}\psi^*(Q+\xi)\right|^2$$

$$x\int d\xi'|\psi(Q+\xi')|^2 \qquad \text{(I.8.)}$$

by the Schwartz inequality[90]. Therefore since $\int dx|\psi(x)|^2 = 1$, (I.8.) implies the desired result, i.e.

$$|F(P,Q)| \leq \left(\frac{1}{\pi\hbar}\right)^N \qquad \text{(I.9.)}$$

In other words the Wigner distribution is strictly contained in the

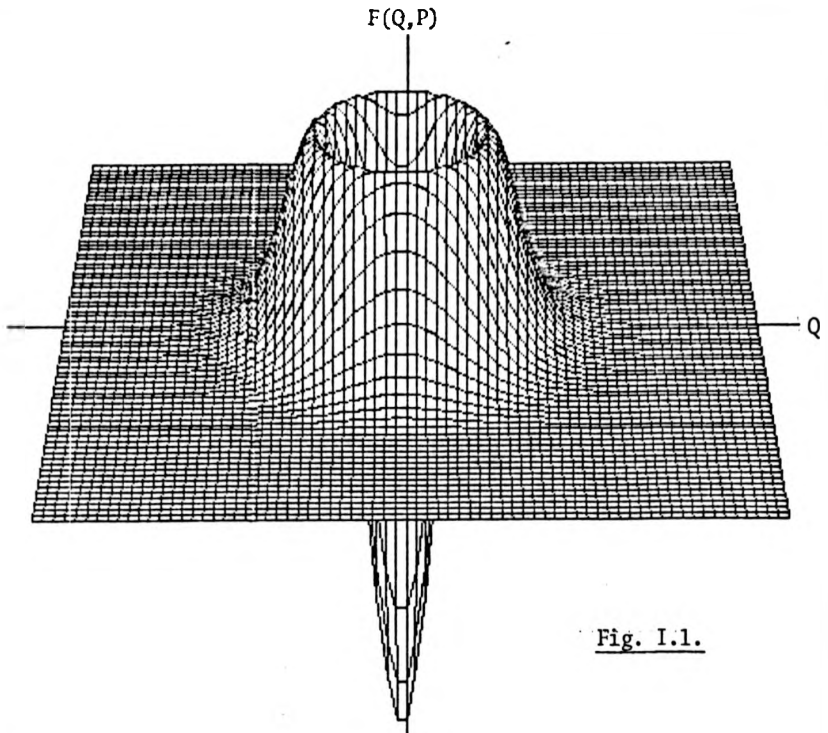

Fig. I.1.

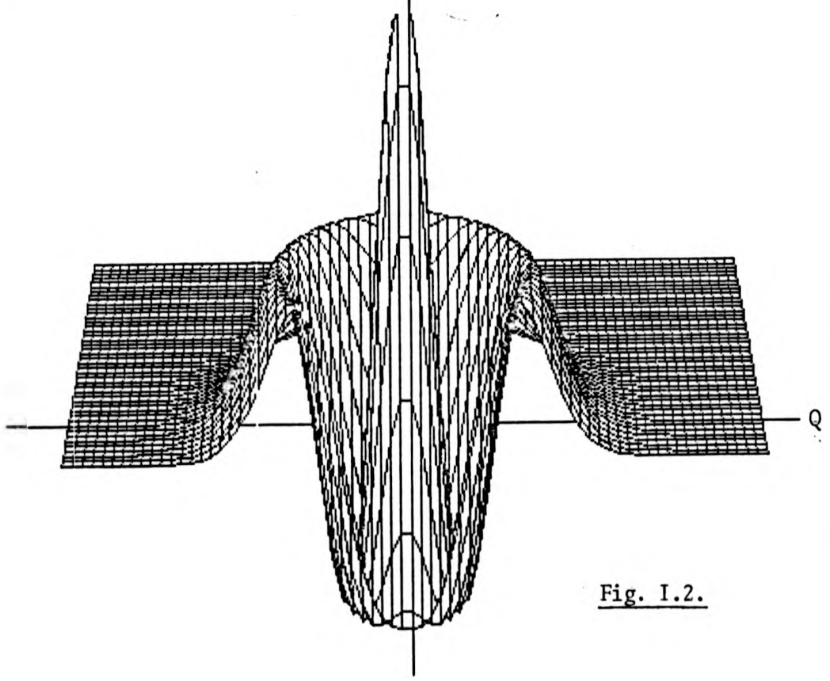

Fig. I.2.

PHASE SPACE PLOTS OF THE WIGNER DISTRIBUTION FOR THE FIRST AND SECOND EXCITED STATES OF THE SIMPLE HARMONIC OSCILLATOR

interval $[-1/(\pi\hbar)^N, 1/(\pi\hbar)^N]$ except perhaps possibly in the classical limit ($\hbar = 0$).

If we now turn our attentions to the Wigner equivalent of an Hermitian quantum operator which may be defined in analogy to (I.2.) as

$$A_W(PQ) = \int d\xi e^{-iP\cdot\xi/\hbar} \langle Q - \frac{\xi}{2}|\hat{A}|Q + \frac{\xi}{2}\rangle$$

$$= \int d\eta e^{iQ\cdot\eta/\hbar} \langle P - \frac{\eta}{2}|\hat{A}|P + \frac{\eta}{2}\rangle \qquad \text{(I.10.)}$$

This correspondence is known as the Wigner-Weyl rule (see for instance references[45][69]) and is equivalent to the one introduced in §3.3.17. where it was shown that combining (I.10.) with the Wigner distribution (I.2.) allows one to calculate the expectation value of an observable through a phase-space integration routine identical to the procedure persued in classical mechanics i.e.

$$\langle A \rangle = \int dPdQF_W(PQt)A_W(PQ) \qquad \text{(I.11.)}$$

Of course differences between quantum and classical mechanics will occur because in general the Wigner equivalent of a quantum operator will not be the same as its' corresponding classical counterpart. However relationships do exist in certain circumstances which are apparent in the following list of properties of Wigner equivalents of Hermitian operators[45]. The important properties are:

$$\text{If } \hat{A} = \text{constant then } A_W(P,Q) = A \qquad \text{(I.12.)}$$

$$\text{If } \hat{A} \equiv \hat{A}(\hat{P}) \text{ then } A_W(P,Q) = A(P) \qquad \text{(I.13.)}$$

$$\text{If } \hat{A} \equiv \hat{A}(\hat{Q}) \text{ then } A_W(P,Q) = A(Q) \qquad \text{(I.14.)}$$

$$\text{Tr } \hat{A} = \left(\frac{1}{2\pi\hbar}\right)^N \int dPdQA_W(P,Q) \qquad \text{(I.15.)}$$

$$\int dP A_W(P,Q) = (2\pi\hbar)^N \langle Q|\hat{A}|Q\rangle \qquad (I.16.)$$

$$\int dQ A_W(P,Q) = (2\pi\hbar)^N \langle P|\hat{A}|P\rangle \qquad (I.17.)$$

There is one additional very important property first due to Groenwald[38] which relates the Wigner equivalent of a product of operators to the individual Wigner equivalents which may be stated as

$$\begin{aligned}[\hat{A}\hat{B}]_W &= A_W(PQ)\exp\left(\frac{\hbar\Omega}{2i}\right)B_W(P,Q) \\ &= B_W(P,Q)\exp\left(\frac{-\hbar\Omega}{2i}\right)A_W(P,Q) \\ &= A_W(Q - \frac{\hbar}{2i}\nabla_P,\ P + \frac{\hbar}{2i}\nabla_Q)B_W(P,Q) \end{aligned} \qquad (I.18.)$$

where $\Omega \equiv \overleftarrow{\nabla}_P\cdot\overrightarrow{\nabla}_Q - \overleftarrow{\nabla}_Q\cdot\overrightarrow{\nabla}_P$ is the Poisson bracket operator (note that $A\Omega B = (A;B)$ is just the standard classical Poisson bracket[36]).

From (I.18.) and (I.15.) we immediately find

$$Tr[\hat{A}\hat{B}] = \left(\frac{1}{2\pi\hbar}\right)^N \int dP dQ A_W(P,Q) B_W(P,Q) \qquad (I.19.)$$

as a natural extension of (I.11.). The importance of (I.18.) stems from the fact that when combined with (I.12.)-(I.14.) it affords a method of calculating the Wigner equivalent of any operator. For instance in considerations of the dynamics of transport across an interface between two semiconductors the electron effective mass should be considered as position dependent leading to a symmetrised kinetic energy operator of the form

$$\hat{H} = \hat{P}\frac{1}{m(Q)}\hat{P} \qquad (I.20.)$$

The Wigner equivalent of this operator is not of the classical $P^2/2m$ form but may be obtained by (I.18.) as follows.

$$
\begin{aligned}
&\left[\hat{P}\,\frac{1}{2m(\hat{Q})}\,\hat{P}\right]_W \\
&= \left(\hat{P}\,\frac{1}{2m(\hat{Q})}\right)_W e^{\frac{\hbar\Omega}{2i}P} \\
&= \left(\frac{1}{2m(\hat{Q})}\right)_W e^{-\frac{\hbar\Omega}{2i}P} e^{\frac{\hbar\Omega}{2i}P} \\
&\equiv \left(\frac{1}{2m(\hat{Q})}\right)_W \{1 - \tfrac{i\hbar}{2}\overleftarrow{\nabla}_Q\}P\{1 + \tfrac{i\hbar}{2}\overrightarrow{\nabla}_Q\}P \\
&= \frac{P^2}{2}\left(\frac{1}{m(\hat{Q})}\right)_W + \frac{\hbar^2}{4}\nabla_Q^2\left(\frac{1}{2m(\hat{Q})}\right)_W
\end{aligned}
\qquad \text{(I.21.)}
$$

which has an additional contribution to the classical form proportional to $\hbar^2$.

It is interesting to note that the classical form is recovered if the function $[1/m(\hat{Q})]_W$ is no more than quadratic in Q so that only the first two moments are involved in its' construction, an effect undoubtedly connected with the Marcinkiewicz theorem (§3.2.).

We can use the property (I.19.) to obtain the final sum rule obeyed by the Wigner distribution by considering the average value of the density matrix itself. Therefore taking $\hat{A} = \hat{B} = \hat{\rho}$ in (I.19.) gives

$$
\begin{aligned}
(2\pi\hbar)^N \int dPdQF_W^2(P,Q) &= \mathrm{Tr}[\hat{\rho}\hat{\rho}] \\
&= \sum_n P_n^2 \\
&\leq 1
\end{aligned}
$$

i.e.

$$
\int dPdQF_W^2(P,Q) \leq \left(\frac{1}{2\pi\hbar}\right)^N \qquad \text{(I.22.)}
$$

and so is square integrable except in the classical limit.

The final piece of information we require concerning the Wigner distribution is the equation of motion it obeys in order that we may study the evolution of the system. This may be obtained from the Liouville equation of motion for the density matrix[43]

$$i\hbar\partial_t\hat{\rho} = [\hat{H},\hat{\rho}]$$

by taking its' Wigner equivalent and using Groenwalds rule (I.18.) to give

$$\partial_t F_W(P,Q,t) = -\left(\frac{2}{\hbar}\right)H_W(PQt)\sin\left(\frac{\hbar\Omega}{2}\right)F_W(PQt) \qquad (I.23.)$$

We note that the semi-classical ($\hbar \to 0$) limit of (I.23.) yields the usual classical Liouville equation for a classical distribution function $f_c(PQ)$[36]

$$\partial_t f_c(P,Q) = -H_W(PQ)\Omega f_c(P,Q)$$

Therefore to conclude, combining all the relevant properties of the Wigner distribution together we see that it is a very useful function from both mathematical and computational aspects: it is real valued, finite, square integrable, normalisable, correct probability distributions are obtained from its' projections and it may be used to calculate expectation values of observables in a manner identical to classical mechanics. Moreover although it has not been discussed in this Appendix because the thesis is restricted to non-relativistic quantum theory, the Wigner distribution may be defined in a covariant form that allows relativistic phenomena to be studied[25]. Therefore the Wigner approach constitutes an overall coherent framework in which classical, quantum and relativistic phenomena may be studied and compared in a more direct fashion than may otherwise be accomplished.

APPENDIX II

GREENS FUNCTIONS DEFINITIONS

The Greens function is a quantum statistical average of an operator $\hat{X}$ defined as the many body trace over the density matrix, i.e.

$$G(X) = \langle\hat{X}\rangle = Tr[\hat{X}\hat{\rho}] \tag{II.1.}$$

In the Heisenberg representation for a time independent Hamiltonian, the time dependence of an operator is given by

$$\hat{X}(t) = \exp[iHt]\hat{X}(t = 0)\exp[-iHt] \tag{II.2.}$$

where the time independent density matrix is taken to be evaluated at time $t = 0$ when the system is in thermal equilibrium and consequently determined by the density matrix in the grand canonical ensemble

$$\rho = \frac{\exp[-\beta(H - \mu N)]}{Tr[\exp[-\beta(H - \mu N)]]} \tag{II.3.}$$

The operators over which we average are usually products of annihilation and creation operators of electrons or phonons defined at different times. In the case of phonons we also use the ion-displacement operator.

Because the operators are defined at different times we use the Wick Time Ordering operator $\hat{T}$[51] which arranges quantities of the earliest times to the right of operators evaluated at subsequent times. In the case of fermions $\hat{T}$ also contains a parity operator which is used dependent on whether the final permutation of operators involves an odd or even number of pairwise commutations. This is best seen by explicit examples.

In what follows an upper sign refers to Bose statistics and the lower sign to fermions, thus (±).

The one-electron Greens function is defined as

$$G(1,1') = \frac{1}{i}\langle\hat{T}\psi(r_1t_1)\psi^\dagger(r_1't_1')\rangle$$

$$= \frac{1}{i}\theta(t_1 - t_1')\langle\psi(r_1,t_1)\psi^\dagger(r_1't_1')\rangle$$

$$\pm \frac{1}{i}\theta(t_1' - t_1)\langle\psi^\dagger(r_1't_1')\psi(r_1t_1)\rangle \qquad \text{(II.4.)}$$

where $\theta(t)$ is the usual step function.

Similarly the two-electron Greens function is defined as

$$G_2(1,1',2,2') = \left(\frac{1}{i}\right)^2\langle\hat{T}\psi(r_1t_1)\psi(r_2t_2)\psi^\dagger(r_2't_2')\psi^\dagger(r_1't_1')\rangle \qquad \text{(II.5.)}$$

Note that the Greens function (II.4.) is composed of two separate analytic branches; one for $t_1 > t_1'$ (in which case $G(1,1')$ is denoted by $G^>(11')$) and the other for $t_1 < t_1'$ (and is denoted by $G^<(1,1')$). It is not defined and is therefore discontinuous for $t_1 = t_1'$.

The two analytic branches are the physically relevant quantities since they are related to the local electron density $n(R,T)$ through

$$n(R,T) \equiv \langle\psi^\dagger(R,t)\psi(R,t)\rangle$$

$$= \pm iG^<(1,1')\Big|_{\substack{r_1=r_1'=R \\ t_1'=t_1+\delta=T}} \qquad \text{(II.6.)}$$

where δ is a positive infinitesimal to ensure the correct sequence of operators within the average.

Similarly

$$iG^>(11') = \langle\psi(1)\psi^\dagger(1')\rangle$$

so

$$iG^>(11')\Big|_{\substack{r_1=r_1'=R \\ t_1=t_1'+\delta=T}} = \langle\psi(RT)\psi^\dagger(R,t)\rangle$$

$$= 1 \pm n(R,t) \qquad \text{(II.7.)}$$

We can also see at this stage that these analytic branches are

are related to the Wigner distribution (Appendix I) since from definition (I.1.)

$$F_W(R,P,T) \equiv \left(\frac{1}{2\pi}\right)^N \int dr e^{-iP\cdot r} \langle \psi^\dagger(R + \frac{r}{2},T)\psi(R - \frac{r}{2},T)\rangle$$

$$= \left(\frac{1}{2\pi}\right)^N \int dr e^{-iP\cdot r} (\pm i) G^<(11') \Big|_{\substack{r_1=R-\frac{r}{2} \\ r_1'=R+\frac{r}{2} \\ t_1'=t_1+\delta=T}} \qquad \text{(II.8.)}$$

$$= \int \frac{d\omega}{2\pi} G^<(R,T,P,\omega) \qquad \text{(II.9.)}$$

where in going from (II.8.) to (II.9.) we have introduced the partial Fourier-Laplace transform on the off-diagonal co-ordinates of the Greens Function as:-

$$G^>(R,T,P,\omega) = \left(\frac{1}{2\pi}\right)^N \int dr dt e^{-iP\cdot r+i\omega t} (i) G^>(1,1') \Big|_{\substack{r_1'=R+\frac{r}{2} \\ r_1=R-\frac{r}{2} \\ t_1'=T+\frac{t}{2} \\ t_1=T-\frac{t}{2}}} \qquad \text{(II.10.)}$$

and

$$G^<(R,T,P,\omega) = \left(\frac{1}{2\pi}\right)^N \int dr dt e^{-iP\cdot r+i\omega t} (\pm i) G^<(1,1') \Big|_{\substack{r_1'=R+\frac{r}{2} \\ r_1=R-\frac{r}{2} \\ t_1'=T+\frac{t}{2} \\ t_1=T-\frac{t}{2}}} \qquad \text{(II.11.)}$$

The sequence of operations performed in obtaining the Fourier-Laplace transformed version of the Greens functions (specifically changing variables from $(r_1,r_1',t_1,t_1') \rightarrow (R,r,T,t)$ and then transforming only on the variables (r,t)) will be collectively referred to as a Wigner transform in this thesis.

It is clear from (II.11.) that the Greens function $G^<(RTP\omega)$ may be considered as a generalisation of the Wigner distribution function (Appendix I and §3.3.) into a phase space characterised by the canonical variables

(R,P,T,ω). Indeed the projection of the Greens function down the energy axis (ω) gives precisely the Wigner distribution (II.9.).

So far the time variables in the Greens functions have been implicitly restricted to the real interval $0 \leq t \leq \infty$. However for non-equilibrium Greens functions this can impose various difficulties concerning the analytic behaviour of the various branches of the real time Greens functions and the choice of integration contours[26][60]. It has been found to be more convenient to work with the analytic continuations of these functions into the imaginary time domain principally because then the Greens functions obey the periodic boundary conditions[51]:

$$G(11')\Big|_{\substack{T=T_0\\t=t_0}} = \pm e^{\beta\mu} G(1,1')\Big|_{\substack{T=T_0-i\beta/2\\t=-(t_0+i\beta)}} \qquad \text{(II.12.)}$$

This identity follows because

$$G^<(T+\frac{t}{2},T-\frac{t}{2})\Big|_{\substack{T=T_0\\t=t_0}} = \pm\left(\frac{1}{i}\right)\langle e^{\beta(H-\mu N)}\psi(T_0-\frac{t_0}{2})e^{-\beta(H-\mu N)}\psi^\dagger(T_0+\frac{t_0}{2})\rangle$$

and since $\psi f(N) \equiv f(N+1)\psi$ this relationship obtained from the cyclic invariance of the trace becomes

$$G^<(11')\Big|_{\substack{T=T_0\\t=t_0}} = \pm\frac{e^{\beta\mu}}{i}\langle[e^{\beta H}\psi(T_0-\frac{t_0}{2})e^{-\beta H}]\psi^\dagger(T_0+\frac{t_0}{2})\rangle$$

$$= \pm\frac{e^{\beta\mu}}{i}\langle\psi(T_0-\frac{t_0}{2}-i\beta)\psi^\dagger(T_0+\frac{t_0}{2})\rangle$$

where we have used (II.2.). This is equivalent to the boundary condition (II.12.)

Therefore if we consider the time variable to be restricted to the imaginary time domain $0 \leq i(t-t_0) \leq \beta$ we may define two analytic branches of the imaginary time Greens function

$$G(1,1') = \begin{cases} G^{>}(11') & \text{for} \quad it_1 > it_1' \\ G^{<}(11') & \text{for} \quad it_1 < it_1' \end{cases} \tag{II.13.}$$

and because of the boundary condition (II.12.) we know that the Fourier-Laplace transforms (II.10.) and (II.11.) are well defined.

All the foregoing discussion applies equally well to the phonon Greens function P(11') defined in terms of phonon annihilation b(1) and creation $b^{\dagger}(1')$ operators as

$$P(11') = \left(\frac{1}{i}\right) \langle \hat{T} b(1) b^{\dagger}(1') \rangle \tag{II.14.}$$

since we have already allowed for bosons by the inclusion of the uppersign.

We note in particular the one-phonon Wigner distribution function $n_W(R,K,T)$ as the projection of the one-phonon Greens function branch $P^{<}(RTK\omega)$ i.e.

$$n_W(R,K,T) = \int \frac{d\omega}{2\pi} P^{<}(R,K,T,\omega) \tag{II.15.}$$

Unfortunately although the phonon Greens function has the greater physical appeal, it is mathematically more convenient to work with a phonon <u>correlation</u> function D(11') which correlates the displacement operators $\hat{q}_k(t)$ at different times and places through the definition

$$D(1,1') = \frac{1}{i} [\langle Tq(1)q^{\dagger}(1') \rangle - \langle q(1) \rangle \langle q^{\dagger}(1') \rangle] \tag{II.16.}$$

The correlation function may be related to the phonon Greens function because the displacement operator is related to the phonon annihilation and creation operators through[60][66]

$$q_k(t) = \left(\frac{1}{2\omega_k \hbar}\right)^{\frac{1}{2}} [b_k + b_{-k}^{\dagger}] \tag{II.17.}$$

where the annihilation and creation operators are taken to obey the anti-commutation relations

$$[b_\lambda, b^\dagger_{\lambda'},]_+ = \hbar\delta_{\lambda,\lambda'} \qquad \text{(II.18.)}$$

Substituting (II.17.) into (II.16.) gives the correlation function as

$$D(1,1') = \left[\frac{1}{2i\hbar\omega_{\frac{k_1+k_1'}{2}}}\right] <T\left[\frac{\omega^2_{\frac{k_1+k_1'}{2}}}{\omega_{k_1}\omega_{k_1'}}\right]^{\frac{1}{2}} [b_{k_1} b^\dagger_{k_1'} + b^\dagger_{-k_1} b_{-k_1'}]> \qquad \text{(II.19.)}$$

It is convenient to change variables $k_1 \to K - \frac{k}{2}$, $k_1' \to K + \frac{k}{2}$ and absorb the factors $\omega_K/\sqrt{\omega_{K-k/2}}$ into $b_{K-k/2}$ and similarly for $\omega_K/\sqrt{\omega_{K+k/2}}$ since the commutation relation (II.18.) is unchanged giving

$$D(K,k,T,t) = \left[\frac{1}{2i\omega_K\hbar}\right] <T[b_{K-k/2}(T + \tfrac{t}{2}) b^\dagger_{K+k/2}(T - \tfrac{t}{2})$$
$$+ b^\dagger_{-K+k/2}(T - \tfrac{t}{2}) b_{-K-k/2}(T + \tfrac{t}{2})]>$$

which may be Fourier transformed to yield

$$D^{\gtrless}(R,T,K,\omega) = \left[\frac{1}{2\hbar\omega_K}\right] [P^{\gtrless}(R,T,K,\omega) + P^{\lessgtr}(R,T,-K,-\omega)] \qquad \text{(II.20.)}$$

The relationship (II.20.) is used in Chapter 4 to covert the equations of motion of the phonon correlation functions to equations for the phonon Greens functions.

The only other Greens function used in this thesis is a mixed Greens function arising from the electron-phonon coupling considered in Chapter 4 and is defined as

$$<T\psi(1)q(2)\psi^\dagger(1')> \qquad \text{(II.21.)}$$

It does not warrant a special symbol since it may be reduced to products of simpler Greens functions and functional derivatives (see Appendix III) and thus may be eliminated from the discussions.

We now come to a quantity of particular importance known as a spectral function.

It has already been noted that Greens functions are discontinuous across the real time axis: they are undefined for $t_1 = t_1'$ and have two distinct analytic branches for $it_1 > it_1'$ and $it_1 < it_1'$. Therefore we would expect that the magnitude of this discontinuity defined as the difference between the two analytic branches in the limit as they both approach the real axis, has some significance in our deliberations. It is this difference that is refered to as a spectral (density) function which is perhaps the most important quantity we would like to evaluate as we will soon see.

The two spectral functions with which we are concerned correspond to the one electron and phonon Greens functions. We consider first the electron case where, by the preceding introduction, the one electron spectral function A(11') is defined as

$$A(1,1') = G^{>}(1,1') - G^{<}(1,1')$$

$$= \frac{1}{i} \langle \psi(1)\psi^{\dagger}(1') \rangle + \frac{1}{i} \langle \psi^{\dagger}(1')\psi(1) \rangle \qquad \text{(II.22.)}$$

which may be Wigner transformed using (II.10.) and (II.11.) to give

$$A(R,T,P,\omega) \equiv \frac{i}{(2\pi)^N} \int drdte^{-iP\cdot r + i\omega t} A(1,1')$$

$$= G^{>}(RTP\omega) + G^{<}(RTP\omega) \qquad \text{(II.23.)}$$

Actually this is not quite rigorous because in the definition of the time transform we need to ensure convergence. Since when we choose to change variables from $(t_1, t_1') \rightarrow (T,t)$ then $G^{>}$ is a function of $+t$ and $G^{<}$ depends on $-t$. Consequently in the transform of $G^{>}$ for example we need ω to have a small positive imaginary component, i.e.

$$G^{>}(\omega) \equiv \int dte^{i(\omega + i\delta)t} iG^{>}(t) = G^{>}(\omega_R + i\delta)$$

and $G^{>}(\omega)$ is defined in the upper half complex plane. Similarly in the definition of $G^{<}(\omega)$ we should have

$$G^{<}(\omega) \equiv G^{<}(\omega_R - i\delta)$$

In other words the spectral function should be strictly defined as

$$A(RTP\omega) = G^{>}(RTP\omega + i\delta) + G^{<}(R,T,P,\omega - i\delta) \qquad \text{(II.24.)}$$

From this definition follows the important consequence that the analytic behaviour of the one-electron Greens function is governed entirely by the spectral function since

$$G(\omega) \equiv \int dt e^{i\omega t} G(1,1')$$

$$= \int dt e^{i\omega t} [\theta(t)G^{>}(t) + \theta(-t)G^{<}(t)] \qquad \text{(II.25.)}$$

$$= \int dt e^{i\omega t} \int \frac{d\omega'}{2\pi} e^{i\omega' t} \left[\frac{G^{>}(t)}{i(\omega' - i\delta)} - \frac{G^{<}(t)}{i(\omega' + i\delta)} \right] \qquad \text{(II.26.)}$$

$$= \int \frac{d\omega'}{2\pi} \left[\frac{G^{>}(\omega')}{\omega - \omega' + i\delta} + \frac{G^{<}(\omega')}{\omega - \omega' - i\delta} \right]$$

$$\equiv \int \frac{d\omega'}{2\pi} \frac{[G^{>}(\omega' + i\delta) + G^{<}(\omega' - i\delta)]}{\omega - \omega'}$$

i.e. $$G(\omega) \equiv \int \frac{d\omega'}{2\pi} \frac{A(\omega')}{\omega - \omega'} \qquad \text{(II.27.)}$$

where we have made use of (II.24.) and in going from (II.25.) to (II.26.) we utilised the θ-function representation

$$\theta(t) = \int_{-\infty}^{t} d\tau \delta(\tau) = \int \frac{d\omega}{2\pi i} \frac{e^{i\omega t}}{\omega - i\delta}$$

(II.27.) is an important representation of a Greens function and is often used to define the spectral function. From this identity follows the relationship that the spectral function is equal to the imaginary part of the Greens function because

$$G(\omega + i\delta) = P\int \frac{d\omega'}{2\pi} \frac{A(\omega')}{\omega - \omega'} - \frac{i}{2} A(\omega)$$

$$G(\omega - i\delta) = P\int \frac{d\omega'}{2\pi} \frac{A(\omega')}{\omega - \omega'} + \frac{i}{2} A(\omega)$$

from which follows

$$A(\omega) = i[G(\omega + i\delta) - G(\omega - i\delta)] \qquad \text{(II.28.)}$$

Therefore if we know an explicit form of the Greens function its' corresponding spectral function may be obtained from (II.28.).

It is clear from the definition (II.23.) that the spectral function is real and moreover it must obey the sum rule

$$\int \frac{d\omega}{2\pi} A(R,T,P,\omega) = 1 \qquad \text{(II.29.)}$$

because from (II.22) and (II.23.)

$$\begin{aligned}\int \frac{d\omega}{2\pi} A(R,T,P,\omega) &= \int \frac{d\omega}{2\pi} \int dt \frac{dr}{(2\pi)^N} e^{i\omega t - iP\cdot r} \langle \psi(1)\psi^\dagger(1') + \psi^\dagger(1')\psi(1)\rangle \\ &= \int \frac{dr}{(2\pi)^N} e^{-iP\cdot r} \langle \psi(r_1,t)\psi^\dagger(r_1',t) + \psi^\dagger(r_1',t)\psi(r_1 t)\rangle \\ &= 1\end{aligned}$$

from the electron commutation relations at equal times.

Similar relationships may be constructed for the phonon spectral function B(1,1') corresponding to the one-phonon Greens function P(1,1') which is defined as

$$\begin{aligned}B(1,1') &= P(t_1 > t_1') - P(t_1 < t_1') \\ &= \frac{1}{i} \langle b(1)b^\dagger(1') - b^\dagger(1')b(1)\rangle \qquad \text{(II.30.)}\end{aligned}$$

which may be Wigner transformed into

$$B(R,T,K,\omega) = P^{>}(R,T,K,\omega) - P^{<}(R,T,K,\omega) \qquad \text{(II.31.)}$$

This phonon spectral function obeys the sum rules

$$\int \frac{d\omega}{2\pi} B(R,T,K,\omega) = 1 \qquad \text{(II.32.)}$$

and

$$\int \frac{d\omega}{2\pi} \omega B(RTK\omega) = \hbar\omega_K \qquad \text{(II.33.)}$$

The first relationship (II.32.) follows for the same reason as in the electron case and (II.33.) may be illustrated as follows. From the definitions (II.30.) and (II.31.)

$$\int \frac{d\omega}{2\pi} \omega B(\omega) \equiv \int \frac{d\omega}{2\pi} dt dk e^{ik\cdot R + i\omega t_\omega} \times$$

$$\times \sum_{m,n} \alpha_m \left[\langle m| e^{\frac{-iHt}{2}} b(T) e^{\frac{iHt}{2}} |n\rangle\langle n| e^{\frac{-iHt}{2}} b^\dagger(T) e^{\frac{iHt}{2}} |m\rangle \right.$$

$$\left. - \langle m| e^{\frac{-iHt}{2}} b^\dagger(T) e^{\frac{iHt}{2}} |n\rangle\langle n| e^{\frac{-iHt}{2}} b(T) e^{\frac{iHt}{2}} |m\rangle \right]$$

$$= \sum_{m,n} \alpha_m \int dk e^{ik\cdot R} (\varepsilon_m - \varepsilon_n) \left[\langle m|b|n\rangle\langle n|b^\dagger|m\rangle \right.$$

$$\left. + \langle m|b^\dagger|n\rangle\langle n|b|m\rangle \right]$$

which may be arranged in the form

$$\int \frac{d\omega}{2\pi} \omega B(\omega) = \int dk e^{ik\cdot R} \langle [[H,b(1)],b^\dagger(1')] \rangle \qquad \text{(II.34.)}$$

However, since $[H,b_K] = \omega_K b_K$ where ω_K is the frequency of a phonon of wavevector K, (II.34.) may be reduced to the form

$$\int \frac{d\omega}{2\pi} \omega B(\omega) = \int dk e^{ik\cdot R} \hbar\omega_{k_1} \delta_{k_1,k_1'}$$

$$= \hbar\omega_K \quad \text{as required.}$$

Of course the phonon correlation function also has an associated spectral function:

$$S_D(\omega) = D^{>}(\omega) - D^{<}(\omega) \tag{II.35.}$$

which must be related to the phonon spectral function B(RTKω) because the correlation and Greens functions are connected through (II.20). It is straightforward to see that this relationship is just

$$S_D(\omega) = \frac{1}{2\hbar\omega_K}\left[B(RTK\omega) - B(R,T,-K,-\omega)\right] \tag{II.36.}$$

Therefore using (II.36.) and sum-rules (II.32.) and (II.33.) it can be seen that the correlation spectral function satisfies the sum rules

$$\int \frac{d\omega}{2\pi} S_D(\omega) = 0 \tag{II.37.}$$

$$\int \frac{d\omega}{2\pi} \omega S_D(\omega) = 1 \tag{II.38.}$$

These five sum rules (II.29.), (II.32.), (II.33.), (II.37.) and (II.38.) are of prime importance since they are identities that must be obeyed if any approximation is made to the spectral function through approximations made in the Greens functions. Much use is made of these sum rules in obtaining the transport equations for electron and phonon Wigner distributions in Chapter 4.

One exceptional situation in which the Greens functions and spectral functions may be obtained <u>exactly</u> is the equilibrium state of free particle systems.

For a free electron

$$\psi^{\dagger}(P,t) = e^{i\varepsilon(P)t}\psi^{\dagger}(P,0) \tag{II.39.}$$

and since the one electron Greens function depends only on the co-ordinate differences $r_1 - r_1'$, $t_1 - t_1'$ we have

$$G(t_1 > t_1') = \frac{1}{i} e^{-\varepsilon(P)t} \langle \psi(P,0)\psi^{\dagger}(P,0) \rangle \tag{II.40.}$$

and similarly

$$G(t_1 < t_1') = \frac{-1}{I} e^{-i\varepsilon(P)t} \langle \psi^\dagger(P,0)\psi(P,0) \rangle \qquad \text{(II.41.)}$$

which gives for the electron spectral function

$$A(P,\omega) = 2\pi\delta(\omega - \varepsilon(P)) \qquad \text{(II.42.)}$$

which clearly obeys the sum rule (II.29.). It can be seen from (II.40.) and (II.41.) that the two branches of the Greens function may be written exactly in the form

$$G^<(P,\omega) = A(P,\omega)f(P) \qquad \text{(II.43.)}$$

$$G^>(P,\omega) = A(P,\omega)[1 - f(P)] \qquad \text{(II.44.)}$$

where $A(P,\omega)$ is given in (II.42.) and $f(P) = \langle \psi^\dagger(P)\psi(P) \rangle$ is the electron distribution function. We note that (II.43.) satisfies the identity (II.9.) if we associate the equilibrium distribution with the Wigner distribution.

We may obtain an explicit form for the equilibrium distribution function $f(P)$ from a special relation connecting the two branches of the Greens function in equilibrium. Specifically from the boundary condition (II.12.), it may be Wigner transformed in equilibrium to give

$$G^<(P,\omega) = e^{-\beta(\omega-\mu)} G^>(P,\omega) \qquad \text{(II.45.)}$$

If we substitute (II.43.) and (II.44.) into this special relationship we find

$$A(P,\omega)f(P) = A(P,\omega)e^{-\beta(\omega-\mu)}[1 - f(P)]$$

To isolate an expression for $f(P)$ we integrate over ω and use the equilibrium spectral function (II.42.) which allows a rearrangement to give

$$f(P) = 1/[1 + \exp\beta\{\varepsilon(P) - \mu\}] \qquad \text{(II.46.)}$$

which is recognisable as the usual equilibrium Fermi-Dirac distribution

function depending on an electrons momentum P and energy $\varepsilon(P)$.

In a similar fashion the phonon Greens function and correlation function may be obtained under an equilibrium free particle assumption since in this case we have

$$b_k^\dagger(t) = e^{i\omega_k t} b_k^\dagger(0)$$

so that

$$P(t_1 > t_1') = \frac{1}{i} e^{-i\omega_k t} \langle b_k(0) b_k^\dagger(0) \rangle \qquad \text{(II.47.)}$$

$$P(t_1 < t_1') = \frac{1}{i} e^{-i\omega_k t} \langle b_k^\dagger(0) b_k(0) \rangle \qquad \text{(II.48.)}$$

and so the corresponding spectral function is given by

$$B(K,\omega) = 2\pi\delta(\omega - \omega_K) \qquad \text{(II.49.)}$$

This spectral function satisfies the two sum rules (II.32.) and (II.33.) as it ought to and may be used to show that the Laplace transform of (II.48.) can be written as

$$P^>(K,\omega) = B(K,\omega)[1 + n(K)] \qquad \text{(II.50.)}$$

$$P^<(K,\omega) = B(K,\omega)n(K) \qquad \text{(II.51.)}$$

where $n(K) = \langle b_K^\dagger b_K \rangle$ is the phonon distribution function corresponding to the equilibrium limit of the phonon Wigner distribution as may be seen by integrating (II.51.) over ω and comparing with (II.15.)

Furthermore we can obtain the explicit expression for this equilibrium phonon distribution by noting that in equilibrium the phonon Greens functions are related by

$$P^<(K,\omega) = e^{-\beta\omega} P^>(K,\omega) \qquad \text{(II.52.)}$$

(This expression is equivalent to the Laplace transform of (II.12.) where we lose the $\exp[\beta\mu]$ term because the average is performed using the canonical ensemble due to the non-conservation of phonons.) Thus substituting (II.50.) and (II.51.) into (II.52.), integrating the expression over ω and making use of the phonon spectral function (II.49.) gives the usual form of the Bose-Einstein distribution for a phonon of wavevector K and frequency ω_K i.e.

$$n(K) = 1/[\exp(\beta\omega_K) - 1] \qquad \text{(II.53.)}$$

This is one of the very few cases where an explicit evaluation of the Greens functions and spectral functions is possible. Once interacting and non-steady state systems are considered we have to resort to idealisations in the transport equations to obtain any analytic results.

Moreover the exact relationships (II.43.), (II.44.), (II.50.) and (II.51.) are no longer identities in non-equilibrium cases. However it is convenient to introduce a decomposition of the Greens function branches into products of spectral functions and distribution functions in non-equilibrium states which may be considered as the definition of non-equilibrium distribution functions. Thus we define

$$G^{<}(R,T,P,\omega) = A(R,T,P,\omega)f(R,T,P) \qquad \text{(II.54.)}$$

$$G^{>}(R,T,P,\omega) = A(R,T,P,\omega)[1 - f(R,T,P)] \qquad \text{(II.55.)}$$

$$P^{<}(R,T,K,\omega) = B(R,T,K,\omega)n(R,T,K,) \qquad \text{(II.56.)}$$

$$P^{>}(R,T,K,\omega) = B(R,T,K,\omega)[1 + n(R,T,K)] \qquad \text{(II.57.)}$$

These decompositions are allowed because they are consistent with all the sum rules and relationships we have introduced so far; thus for example from (II.9.) we must have

$$\int \frac{d\omega}{2\pi} G^{<}(R,T,P,\omega) = f(R,T,P)$$

which is certainly obtained by (II.54.) if we use the normalisation sum rule of the spectral function (II.29.). Of course these non-equilibrium relationships ensure that the correct behaviour is obtained in the equilibrium limit in that the exact relationships (II.43.), (II.44.), (II.50) and (II.51.) are reproduced. Thus the non-equilibrium distributions defined through the consistency relations (II.54.)-(II.57.) are precisely the Wigner electron and phonon distributions.

There is one final comment regarding the use of Greens functions in this thesis: so far they have been expressed in the Heisenberg representation, but to exploit the functional derivative technique to the full, as attempted in Chapter 4, it is useful to convert the imaginary time Greens functions into the interaction representation which allows a functional isolation of the external driving field as follows.

We assume that at $t = 0$ our system is in thermal equilibrium at which time the sudden application of external fields drives the system out of equilibrium. In the Heisenberg representation the density matrix is time independent and satisfies a Bloch equation[102]

$$-\frac{\partial \rho}{\partial \beta} = (H - \langle H \rangle)\rho \qquad \text{(II.58.)}$$

which has a structural similarity to the Schrödinger equation but where β corresponds to an imaginary time $\tau = -i\hbar\beta$.

If we decompose the Hamiltonian into a field free part H_0 and a part V which contains the explicit effects of the external driving fields we may transform (II.58.) into an interaction picture where the corresponding density matrix ρ_I is related to the Heisenberg density matrix through[102]

$$\rho_I = e^{\beta(H_0 - \langle H \rangle)}\rho$$

which satisfies the equation

$$\frac{\partial \rho_I}{\partial \beta} = -V_I \rho_I \tag{II.59.}$$

with the boundary condition $\rho_I(t = 0) = \rho$ and where

$$V_I = e^{\beta(H_0 - \langle H \rangle)} V e^{-\beta(H_0 - \langle H \rangle)} \tag{II.60.}$$

Equation (II.59.) corresponds to the usual real time equation of motion in the interaction representation ($\hbar = 1$):

$$\partial_\tau \rho_I = -iV_I \rho_I \tag{II.61.}$$

where τ is considered to be the imaginary quantity $-i\beta$. Since this equation has the formal solution

$$\rho_I(\tau) = \rho(0)\hat{T}\exp[-i \int_0^\tau d\tau' V_I(\tau')]$$

we have the imaginary time formalism

$$\rho_I = \rho(0)\hat{T}\exp[-i \int_0^{-i\beta} d\tau V_I(\tau)] \tag{II.62.}$$

This density matrix may be used to define averages in the interaction picture for imaginary times as

$$\langle \hat{O} \rangle = \frac{Tr[\hat{\rho}\hat{O}]}{Tr[\hat{\rho}]} = \frac{Tr[\rho(0)\hat{T}\hat{S}\hat{O}]}{Tr[\rho(0)\hat{T}\hat{S}]} = \frac{\langle \hat{T}\hat{S}\hat{O} \rangle_0}{\langle \hat{T}\hat{S} \rangle_0} \tag{II.63.}$$

where the imaginary time S-matrix is defined as

$$S = \exp[-i \int_0^{-i\beta} d\tau V(\tau)] \tag{II.64.}$$

and the notation $\langle --- \rangle_0$ in (II.63.) refers to the average being performed in the Heisenberg representation at $t = 0$ where $\rho \equiv \rho(H_0)$.

The form (II.63) is particularly convenient for use with functional derivative techniques since it manages to isolate the explicit field dependence into the S-matrix (II.64.) which is why it is the prefered representation used in Chapter 4 where $V(\tau)$ is given by

$$V(\tau) \propto \int dr_2[V(r_2,\tau)n(r_2,\tau) + J(r_2,\tau)q(r_2,\tau)]$$

for external electric (V) and pressure (J) fields coupled directly to the electron density (n) and ion displacements (q) respectively.

APPENDIX III

FUNCTIONAL DERIVATIVE IDENTITIES

One of the more convenient aspects of working with Greens functions in the imaginary time domain in the interaction representation is that we can obtain a set of analytical relationships concerning the functional change of a Greens function with respect to an incremental change in the driving field often useful in iterative expansions.

To illustrate we take the situation of the one electron Greens function defined through the interaction representation (II.63.) in imaginary time formalism as

$$G(1,1') = \frac{1}{i} \frac{\langle TS\psi(1)\psi^{\dagger}(1')\rangle}{\langle TS\rangle} \qquad \text{(III.1.)}$$

where

$$S = \exp -i \int_0^{i\beta} d2[V(2)n(2) + J(2)q(2)] \qquad \text{(III.2.)}$$

where J,V are the perturbations (not considered to be small) and n(2), q(2) represent the system operators of interest. (III.1.) is the definition of a one electron Greens function appropriate to the model considered in Chapter 4.

We may consider the functional change in the S-matrix (III.2.) due to an incremental change in the driving fields i.e. $V(2) \rightarrow V(2) + \delta V(2)$, $J(2) \rightarrow J(2) + \delta J(2)$ given as

$$\delta S = S \times \frac{1}{i} \int_0^{i\beta} d2[n(2)\delta V(2) + q(2)\delta J(2)] \qquad \text{(III.3.)}$$

This would lead to a functional variation of the Greens function (III.1.) through

$$\delta G(1,1') \equiv \frac{1}{i}\left[\frac{\langle T\delta S\psi(1)\psi^{\dagger}(1')\rangle}{\langle TS\rangle} - \frac{\langle T\delta S\rangle}{\langle TS\rangle}\frac{\langle TS\psi(1)\psi^{\dagger}(1')\rangle}{\langle TS\rangle}\right]$$

$$= \int_0^{-i\beta} d2\left\{\pm\left[\left(\frac{1}{i}\right)^2 \frac{\langle TS\psi(1)\psi(2)\psi^{\dagger}(2^+)\psi^{\dagger}(1')\rangle}{\langle TS\rangle}\right.\right.$$

$$\left. - \frac{\langle TS\psi(1)\psi^{\dagger}(1')\rangle}{i\langle TS\rangle}\frac{\langle TS\psi(2)\psi^{\dagger}(2^+)\rangle}{i\langle TS\rangle}\right]\delta V(2)$$

$$+ \left[\left(\frac{1}{i}\right)^2 \frac{\langle TS\psi(1)q(2)\psi^{\dagger}(1')\rangle}{\langle TS\rangle}\right.$$

$$\left.\left. - \frac{\langle TS\psi(1)\psi^{\dagger}(1')\rangle}{i\langle TS\rangle}\frac{\langle TSq(2)\rangle}{i\langle TS\rangle}\right]\delta J(2)\right\} \qquad \text{(III.4.)}$$

which upon using the Greens functions definitions (III.1.), (II.5.) and (II.21.) may be expressed in the form

$$\delta G(1,1') = \int_0^{-i\beta}\left\{\pm[G_2(11'22^+) - G(11')G(22^+)]\delta V(2)\right.$$

$$\left. + \left[\left(\frac{1}{i}\right)^2 \frac{\langle TS\psi(1)q(2)\psi^{\dagger}(1')\rangle}{\langle TS\rangle} - \frac{1}{i}Q(2)G(1,1')\right]\delta J(2)\right\} \qquad \text{(III.5.)}$$

The above construction allows us to associate the functional derivative of G(1,1') with respect to V or J by the respective coefficients in the integral, i.e. we have

$$\frac{\delta G(1,1')}{\delta V(2)} = \pm[G_2(11'22^+) - G(11')G(22^+)] \qquad \text{(III.6.)}$$

$$\frac{\delta G(11')}{\delta J(2)} = \frac{1}{i}\left[\frac{1}{i}\frac{\langle TS\psi(1)q(2)\psi^{\dagger}(1')\rangle}{\langle TS\rangle} - Q(2)G(11')\right] \qquad \text{(III.7.)}$$

An identical procedure leads to the definitions of the functional derivatives of the phonon displacement function Q(1) with respect to the electric and pressure fields, the results of which are

$$\frac{\delta Q(1)}{V(2)} = \left[\frac{\langle TS\psi(2)q(1)\psi^{\dagger}(2^+)\rangle}{i\langle TS\rangle} - Q(1)G(2,2^+)\right] \qquad \text{(III.8.)}$$

$$\frac{\delta Q(1)}{\delta J(2)} = \frac{1}{i}\left[\frac{\langle TSq(1)q(2)\rangle}{\langle TS\rangle} - Q(1)Q(2)\right] \qquad \text{(III.9.)}$$

$$\equiv D(1,2) \text{ by definition (II.16.)}$$

Moreover comparing (III.7.) with (III.8.) gives a relationship connecting the functional derivative of the electron Greens function with respect to the pressure field with the functional derivative of the ion displacement with respect to the electric field as

$$\frac{1}{i}\frac{\delta Q(1)}{\delta V(2)} = \pm \frac{\delta G(22^{+})}{\delta J(1)} \qquad \text{(III.10.)}$$

That a relationship such as (III.10.) exists is not surprising since within the confines of the model of Chapter 4 a variation in the pressure field can only induce a local electron density fluctuation by the intermediary response of the electron-phonon interaction, and similarly the electric field acts on the phonons only indirectly via the electrons. Thus (III.10.) may be viewed as a mathematical expression of this symmetry.

As may be seen in (III.6.)-(III.9.), the functional derivative technique allows two particle Greens functions to be reduced to products of one particle Greens function plus the functional derivatives of the one particle functions. In this sense the functional derivatives are considered as true correlation functions.

APPENDIX IV

THE NON-LOCAL DIFFERENTIAL DRIVING TERM

This appendix obtains exact integro-differential forms for the driving terms in the electron and phonon Wigner distribution transport equations derived in Chapter 4 which compare with the conventional driving term structures of the Boltzmann equation.

Considering the electron driving term first, from §4.3.13. we have

$$DT(\omega) = \int drdt e^{i\omega t - iP\cdot r} g^{<}(R,T,r,t)$$

$$x\ [V(R + \frac{r}{2},T - \frac{t}{2}) - V(R - \frac{r}{2},T + \frac{t}{2})] \qquad (IV.1.)$$

By introducing a δ-function and its' Fourier representation this may be written

$$DT = \int drdtdr'dt' \frac{dk'd\omega'}{(2\pi)^4} V(r',t')g^{<}(r,t)e^{i\omega t - iP\cdot r}$$

$$x\ [e^{-ik'\cdot(R-r'+\frac{r}{2})+i\omega'(T-\frac{t}{2}-t')}$$

$$- e^{ik'\cdot(R-r'-\frac{r}{2})-i\omega'(T+\frac{t}{2}-t')}]$$

$$= \int dr'dt' \frac{dk'd\omega'}{(2\pi)^4} V(R + r',T + t')[e^{ik'\cdot r' - i\omega' t'} - c.c.]$$

$$x \int drdt e^{it(\omega - \frac{\omega'}{2}) - ir(P + \frac{k'}{2})} g^{<}(r,t)$$

$$= \int dr'dt' \frac{dk'd\omega'}{(\pi)^4} V(R + r',T + t')(-2i)\sin 2[k'\cdot r' + \omega'\cdot t']$$

$$x\ g^{<}(R,T,P + k',\omega + \omega') \qquad (IV.2.)$$

where in (IV.2.) we have made use of the definition (II.11.)

To convert (IV.2.) into the driving term for the Wigner distribution function we first integrate over ω, use the identities $\int d\omega \sin\omega t = 0$, $\int d\omega \cos 2\omega t = \pi\delta(t)$ and the relationship (II.9.) to reduce (IV.2.) to the form

$$\int \frac{d\omega}{2\pi} DT(\omega) = \frac{-2}{\pi^3} \int dr'dk'V(R + r',T)\sin[2k'\cdot r']f(R,T,P + k') \qquad (IV.3.)$$

This is still not quite of the desired form but may be transformed by integrating by parts twice as follows:

First with respect to r' if we assume that the potential drops off sufficiently rapidly as $R \to \infty$ we find

$$\int \frac{d\omega}{2\pi} DT(\omega) = \frac{-2}{\pi^3} \int dr'dk' \frac{\partial V}{\partial r'} (R + r',T) \frac{\cos 2k'r'}{2k'} f(R,T,P + k') \qquad (IV.4.)$$

Secondly with respect to p', as long as the Wigner distribution tends to zero at the momenta extrema, (IV.4.) becomes

$$\int \frac{d\omega}{2\pi} DT(\omega) = \frac{1}{\pi^3} \int dr'dk' \frac{\partial V}{\partial r'} (R + r',T)ci[2k'r'] \frac{\partial f}{\partial k'} (R,T,P + k') \qquad (IV.5.)$$

where ci(x) is the cosine inegral function[2] defined as

$$ci(x) = -\int_x^\infty \frac{\cos\tau}{\tau} d\tau$$

which is plotted in Figure (IV.1.).

This integro-differential expression (IV.5.) corresponds to the usual driving term $F\cdot\partial f/\partial p$ in the Boltzmann equation but in this quantum mechanical case the derivatives are evaluated at displaced values of position and momentum jointly weighted by the cosine integral and them summed over all possible position and momentum values. This is in stark contrast to the usual local evaluation of the driving term and is of course a consequence of the uncertainty relations applied to the position and momentum variables in quantum mechanics. Therefore we might expect that the $\hbar \to 0$ limit of (IV.5.) would give the classical expression. Since (IV.5.) has been evaluated in units of $\hbar = 1$ it is necessary to first insert the explicit $\hbar$ dependence in

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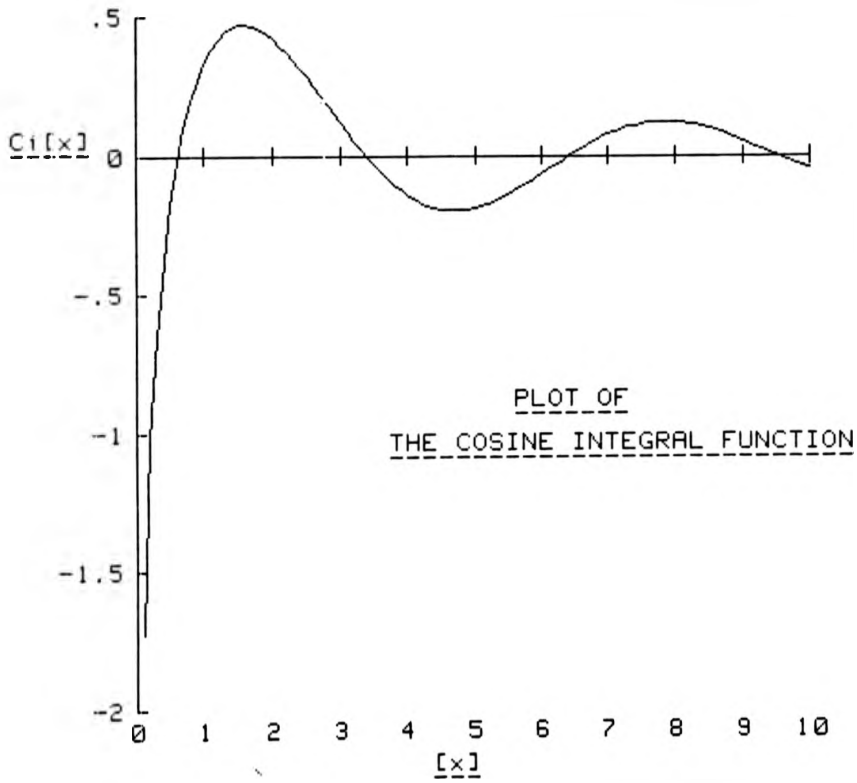

.5
Ci[x]
0
-.5
-1
-1.5
-2
0
1
2
3
4
5
6
7
8
9
10
[x]
PLOT OF
THE COSINE INTEGRAL FUNCTION

Fig. IV.1.

(IV.5.) to give

$$\int \frac{d\omega}{2\pi} DT(\omega) = \frac{1}{(\pi\hbar)^3} \int dr'dk' \frac{\partial V}{\partial r'} (R + r',T) \frac{\partial f}{\partial k'} (R,T,P + k')ci\left[\frac{2k'r'}{\hbar}\right] \tag{IV.6.}$$

which upon changing the variables isolates the $\hbar$ dependence in the potential term only as

$$\int \frac{d\omega}{2\pi} DT(\omega) = \frac{1}{(\pi)^3} \int dr'dk' \frac{\partial V}{\partial r'} (R + \hbar r',T) \frac{\partial f}{\partial k'} (R,T,P + k')ci[2k'r'] \tag{IV.7.}$$

Thus taking the $\hbar \to 0$ limit of (IV.7.) gives

$$\frac{1}{\pi^3} \frac{\partial V}{\partial R} (R,T) \int dk' \frac{\partial f}{\partial k'} (R,T,P + k') \int dr'ci[2k'r'] \tag{IV.8.}$$

To reduce this expression any further requires the following properties of the cosine integral.

Since

$$d_x ci[\alpha x] = -d_x \int_\alpha^\infty \frac{\cos t}{t} dt = \frac{\cos\alpha x}{x}$$

then

$$\begin{aligned} \int_{-\infty}^{\infty} dx ci[\alpha x] &= -\int_{-\infty}^{\infty} dx x d_x ci[\alpha x] \\ &= -\int_{-\infty}^{\infty} dx \cos\alpha x \\ &= -2\pi\delta(\alpha) \end{aligned} \tag{IV.9.}$$

whereupon using this representation of a δ-function in (IV.8.) gives

$$\int \frac{d\omega}{2\pi} DT(\omega) = \frac{-\partial V}{\partial R} (R,T) \frac{\partial f}{\partial P} (R,T,P) \tag{IV.10.}$$

which is just the classical driving term we would expect for a driving field $F = eE = -e\nabla V$.

In general though as may be seen from Figure (IV.1.) and (IV.6.), although the cosine integral weights the local classical term as a dominant contribution, additional quantum corrections occur at alternating positive

and negative peaks on constant phase-space hyperbolae away from the classical trajectory.

In a similar fashion the corresponding driving terms in the phonon distribution transport equation should also involve this cosine integral. Thus starting from the expression given in §4.4.4. in terms of the phonon correlation function, i.e.

$$DT = [\Omega^2(K + \frac{k}{2}) - \Omega^2(K - \frac{k}{2})]D^<(K,k,T,t) \qquad (IV.11.)$$

then we may Wigner transform using the definition

$$D^<(RTK\omega) = \int \frac{dkdt}{(2\pi)^3} e^{i\omega t + ik\cdot R}(i)D^<(K,k,T,t) \qquad (IV.12.)$$

to give

$$DT = -i \int \frac{dkdk'}{(2\pi)^3} \Omega^2(K + k')[\delta(k' - \frac{k}{2}) - \delta(k' + \frac{k}{2})]D^<(K,k,T,\omega) \qquad (IV.13.)$$

Using the Fourier representation of the δ-function, and definition (IV.12.), (IV.13.) is rewritten as

$$DT = \frac{-2}{\pi^3} \int dr'dk'\Omega^2(K + k')\sin[2r'k']D^<(K,T,\omega,R + r') \qquad (IV.14.)$$

which may be integrated by parts, twice, as in the electron case to give finally

$$DT = \frac{1}{(\pi\hbar)^3} \int dr'dk' \frac{\partial\Omega^2}{\partial k'}(K + k') \frac{\partial D^<}{\partial r'}(K,T,\omega,R + r')ci\left[\frac{2r'k'}{\hbar}\right] \qquad (IV.15.)$$

where we have chosen to exhibit the explicit $\hbar$ dependence and ci[x] is the same cosine integral introduced previously. Using the properties of the cosine integral (IV.9.) we may similarly take the $\hbar \to 0$ classical limit of this non local phonon driving term giving

$$DT(\not{h} \to 0) = -\partial_K \Omega^2(K)\, \partial_R D^<(RTK\omega)$$

$$= -2\Omega_K v(K)\, \partial_R D^<(RTK\omega) \qquad \text{(IV.16.)}$$

where $v(K) \equiv \partial\Omega(K)/\partial K$ is the bare phonon group velocity. The $v\cdot\partial_R$ structure in (IV.16.) is as we would have guessed using semiclassical theory and (IV.16.) is explicitly used as the approximation in Chapter 4.

APPENDIX V

HIGHER ORDER CONTRIBUTIONS TO THE ELECTRON SELF ENERGY

In §4.7. the exact expression for the electron self energy

$$\Sigma(1,1') = i\phi_s(1,1')G(1,1') + i\int d2d3\phi_s(1,2)G(1,3)\frac{\delta\Sigma(31')}{\delta V_{eff}(2)} \qquad (V.1.)$$

was approximated by neglecting the functional derivative of the self energy with respect to the effective driving potential.

This appendix shows how it is possible to go beyond this approximation using the local-homogeneity-approximation by recalling the definition of the self energy in terms of the average of an operator $\hat{\Sigma}(1,1')$ i.e.

$$\Sigma(1,1') = \frac{\langle TS\hat{\Sigma}(1,1')\rangle}{i\langle TS\rangle} \qquad (V.2.)$$

where

$$S = \exp - i\int_{t_o}^{t_o-i\beta} d2V_{eff}(2)\psi^{\dagger}(2^{+})\psi(2) \qquad (V.3.)$$

The definition of the S-matrix in (V.3.) is in terms of the effective field since the equations of motion of the electron Greens function, when written in the interaction representation would have a perturbing potential of V_{eff} and not the externally applied potential. Therefore considering the functional variation of the self energy with respect to this effective potential we find

$$\frac{\delta\Sigma(3,1')}{\delta V_{eff}(2)} = \pm[\Sigma_2 - \Sigma(3,1')G(2,2^{+})] \qquad (V.4.)$$

where

$$\Sigma_2 = \left[\frac{1}{i}\right]^2 \frac{\langle TS\psi(2)\psi^{\dagger}(2')\hat{\Sigma}(3,1')\rangle}{\langle TS\rangle}$$

is the equivalent of the two-particle Greens function involving still higher order correlations.

The approximation in Chapter 4 involved assuming that the self energy correlations were zero, i.e. assuming $\delta\Sigma/\delta V_{eff} = 0$. We now assume that these extra correlations may be approximated by $\Sigma(1,2)G(3,3^+)$ and so we neglect Σ_2 above, in which case the closed self energy expression (V.1.) becomes

$$\Sigma(1,1') = i\phi_s(1,1')G(1,1') \mp i \int d2d3\phi_s(1,2)G(2,2^+)G(1,3)\Sigma(3,1') \qquad (V.5.)$$

This integral equation may be converted into an algebraic equation by using the local-homogeneity-approximation and taking a Wigner transform as follows.

The problem term in (V.5.) is

$$\int d3G(1,3)\Sigma(3,1') \int d2\phi_s(1,2)iG(2,2^+) \qquad (V.6.)$$

But $\pm iG(2,2^+) = n(r_2,t_2)$ is the local electron density and under the local-homogeneity-approximation

$$\begin{aligned}\int d2\phi_s(1,2)n(2) &\equiv \int dr_2dt_2\phi_s(r_1 - r_1' - r_2, \frac{r_1 + r_1'}{2} + \frac{r_2}{2}, \\ &\qquad t_1 - t_1' - t_2, \frac{t_1 + t_1'}{2} + \frac{t_2}{2}) \\ &\quad x\ n(r_2 + r_1', t_2 + t_1') \\ &\approx n(R,T) \int dr_2dt_2\phi_s(r_2,R,t_2,T) \\ &= n(R,T)\langle\phi_s(R,T)\rangle \qquad (V.7.)\end{aligned}$$

where $\langle\phi_s(R,T)\rangle = \int dpd\omega\phi_s(R,T,P,\omega)$ is the mean contribution of the <u>effective</u> interaction potential at a point R at time T. This is highly reminiscent of the homogeneous Hartree approximation considered in §4.6. where the electron was considered a free particle but with an additional mean Hartree energy $\varepsilon_H = nV$ where $V = \int drV(r)$ is the total contribution of the <u>bare</u> Coulomb potential. In this case we have a locally homogeneous situation where we have a contribution derived not from the bare interaction but from the screened Coulomb interaction.

Substituting (V.7.) into (V.6.) under the local-homogeneity-approximation, we have

$$n(R,T)\langle\phi_s(R,T)\rangle \int d3G(1 - 3, \frac{1 + 3}{2})\sum(3 - 1', \frac{3 + 1'}{2})$$

$$\simeq n(R,T)\langle\phi_s(R,T)\rangle \int dr_3 dt_3 G(r - r_3, R, t - t_3, T)$$

$$x \sum(r_3, R, t_3, T)$$

which may be Wigner transformed to give

$$n(R,T)\langle\phi_s(R,T)\rangle G(R,T,P,\omega)\sum(R,T,P,\omega) \qquad (V.8.)$$

Using (V.8.) in the Wigner transform of (V.5.) gives the new approximate form of the two branches of the electron self energy as

$$\sum^{\gtrless}(R,T,P,\omega) = (1 + n(R,T)\langle\phi_s(R,T)\rangle G^{\gtrless}(RTP\omega))^{-1} x$$

$$x \int dp' d\omega' \phi_s^{\gtrless}(p - p', \omega - \omega', R, T) G^{\gtrless}(R,T,p',\omega') \qquad (V.9.)$$

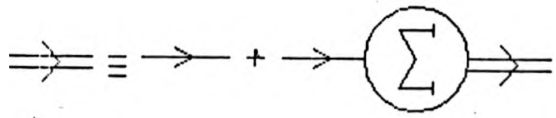
This expression corresponds precisely to the one obtained in Chapter 4 apart from a renormalisation factor $(1 + n(R,T)\langle\phi_s(R,T)\rangle G^{\gtrless}(R,T,P,\omega))^{-1}$.

Therefore it would be straightforward to continue in the manner of Chapter 4 to obtain an electron Wigner distribution equation of motion which would contain these higher order self energy correlations. However, although from the renormalisation factor we see that to include these effects would be to reduce the randomising effects of collisions we would anticipate any such changes would be small because the mean potential evaluated in (V.7.) is the mean of the screened interaction potential which we would imagine to be very small compared to, say, the mean Hartree potential.

The approximation may be given a diagramatic expansion as follows. Since we have

$$G(1,1') = G_0(1,1') + \int d\bar{1}d\bar{2}G_0(1\bar{2})\Sigma(\bar{2}\bar{1})G(\bar{1}1')$$

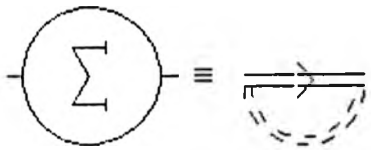
which may be represented by diagrams as



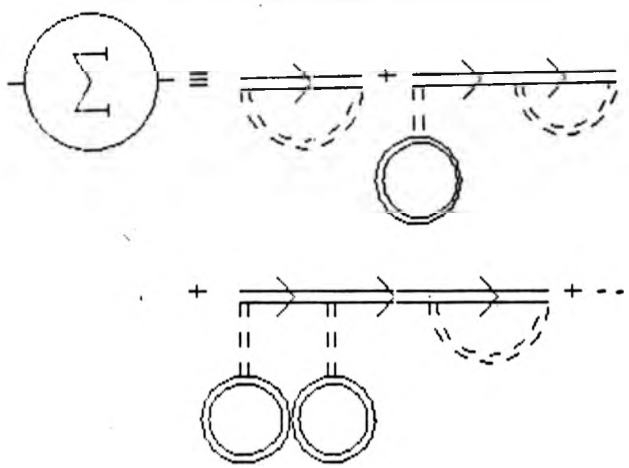
where for the level of approximation used in Chapter 4

$$\Sigma(1,1') = i\phi_s(1,1')G(1,1')$$

i.e.



and for the further correlations considered in this appendix the self energy is given by (V.5.) which has the diagramatic expansion



The strength of the local-homogeneity lies in its' use of approximately summing this infinite series of diagrams to yield the simpler expression (V.9.).

No calculations have been performed yet to ascertain under what

conditions these extra correlations may become significant. We can presume though that since they are correlations specifically connected with a collision process as perhaps defined by an effective screening radius, they should only become important as we tend to low density systems in which the long range Coulomb interaction should induce complicated macroscopic correlations. Therefore for the high density systems of interest in submicron devices the approximation taken in Chapter 4 should be sufficiently accurate to obtain an adequate transport equation.

APPENDIX VI

THE PLASMA DISPERSION FUNCTION AND ITS' PADÉ APPROXIMANT

In the study of wave propagation in a plasma where the electron distribution is determined by a Maxwellian, it is often necessary to consider the properties of an analytic function known as the Plasma Dispersion Function, Z, of complex argument, w. The properties and values of this function have been extensively tabulated in the book of Fried and Conte[32] and this appendix lists the relevant properties required in Chapter 5.

From its' definition

$$Z(w) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{e^{-t^2} dt}{t - w} \qquad \text{(VI.1.)}$$

the plasma (dispersion) function is $\sqrt{\pi}$ times the Hilbert transform of the Gaussian and consequently is a complex valued quantity of complex argument.

Several properties follow directly from (VI.1.), specifically.

$$Z(0) = i\sqrt{\pi} \qquad \text{(VI.2.)}$$

$$Z(w^*) = -[Z(-w)]^* \qquad \text{(VI.3.)}$$

It may also be seen that it satisfies the differential equation

$$Z'(w) = -2[1 + wZ(w)] \qquad \text{(VI.4.)}$$

subject to the initial condition (VI.2.). For real argument, the behaviour of the plasma function for small and large w_R is governed respectively by:

$$Z(w_R) = i\sqrt{\pi}\, e^{-w_R^2} - 2w_R\left(1 - \frac{2w_R^2}{3} + \frac{4w_R^4}{15} + \ldots\right) \qquad \text{(VI.5.)}$$

$$Z(w_R) = i\sqrt{\pi}\, e^{-w_R^2} - \frac{1}{w_R}\left(1 + \frac{1}{2w_R^2} + \frac{3}{4w_R^4} + \ldots\right) \qquad \text{(VI.6.)}$$

which follow from the general relation

$$Z(w_R) = i\sqrt{\pi}\, e^{-w_R^2} - 2e^{-w_R^2}\int_0^{w_R} e^{t^2} dt \qquad \text{(VI.7.)}$$

For the numerical requirements of Chapter 5, it is convenient to use a simple algebraic expression approximating the plasma function (VI.1.) which we now derive.

We assume that the plasma function may be adequately represented by a two-pole Padé approximant[5], that is to say Z(S) may be expressed as the ratio of two polynomials:

$$Z(S) \simeq \frac{P(S)}{Q(S)} = \frac{P_0 + P_1 S}{1 + q_1 S + q_2 S^2} \qquad \text{(VI.8.)}$$

where the four coefficients (P_0, P_1, q_1, q_2) have to be determined by exploiting the properties of the exact plasma function.

Thus by using the 'Hermitian' nature of Z(S) (VI.3.) applied to (VI.8.) we find

$$[Z(-S)]^* = \frac{p_0^* - p_1^* S^*}{1 - q_1^* S^* + q_2^* (S^*)^2}$$

and

$$-Z(S^*) \quad \frac{-p_0 - p_1 S^*}{1 + q_1 S^* + q_2 (S^*)^2}$$

which, upon comparing coefficients in these two expressions, gives the result that the coefficients (p_0, q_1) are purely imaginary and $(p_1 q_2)$ are purely real. Thus, in terms of real coefficients (P_0, P_1, Q_1, Q_2) (VI.8.) becomes:

$$Z(S) = \frac{iP_0 + P_1 S}{1 + iQ_1 S + Q_2 S^2} \qquad \text{(VI.9.)}$$

We may easily see that the boundary condition on the plasma function (VI.2.) implies that

$$P_0 = \sqrt{\pi} \qquad \text{(VI.10.)}$$

The remaining coefficients are determined by requiring that (VI.9.) satisfy the power series (VI.5.) and asymptotic (VI.6.) expansions and that it satisfies the differential equation (VI.4.).

Now for small S, (VI.9.) has the expansion

$$Z(S) \simeq iP_0 + (P_1 - P_0Q_1)S$$

which, upon comparing with (VI.5.) yields the relationships

$$P_0 = \sqrt{\pi} \quad \text{(which we already know)}$$

and

$$P_0Q_1 + P_1 = -2 \tag{VI.11.}$$

Similarly, for large S comparing (VI.6.) with the expansion of (VI.9.) gives the relationship

$$P_1 = -Q_2 \tag{VI.12.}$$

Therefore from (VI.11.) and (VI.12.) we see that the Padé approximant (VI.9.) is governed only by the one variable Q_2 i.e.

$$Z(S) = \frac{i\sqrt{\pi} - Q_2S}{1 - i\left[\frac{2 - Q_2}{\sqrt{\pi}}\right]S + Q_2S^2} \tag{VI.13.}$$

To determine this remaining parameter uniquely we demand the real part of (VI.13.) obeys the differential equation (VI.4.) at its' turning point so that $SReZ(S) = -1$. Using the approximate form (VI.13.) in this differential equation identity leads us to consider a quadratic equation in Q_2, specifically in order for (VI.13.) to satisfy $sReZ(s) = -1$, then Q_2 has to be determined by

$$\frac{S^2}{\pi} Q_2^2 + (2S^2 - \frac{4S^2}{\pi})Q_2 + (1 + \frac{4S^2}{\pi} - 2S^2) = 0$$

i.e.

$$Q_2 = -(\pi - 2) \pm \sqrt{[(\pi - 2)^2 - (\frac{\pi}{S^2} + 4 - 2\pi)]} \qquad \text{(VI.14.)}$$

This is clearly not a unique solution for Q_2 since it depends on the value of S used and thus, unless we specify the value of S at which $Z'(S) = 0$ the parameter Q_2 remains indeterminate. It is forced to be unique by demanding that the square root in (VI.14.) is zero which fixes the value of S at which $Z'(S) = 0$. If this particular value of S is not reasonably close to the true value of the turning point, then the $\frac{1}{2}$ Padé approximant considered here would not be appropriate and we would need to consider a better approximation. Fortunately this is not necessary as we will soon see.

Consequently, demanding a unique solution for Q_2 gives

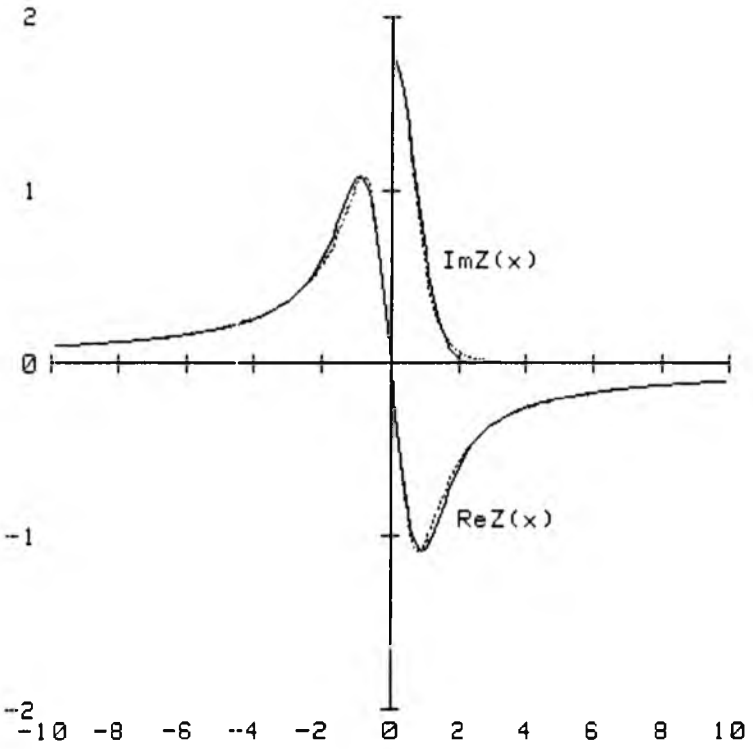
$$Q_2 = 2 - \pi \qquad \text{(VI.15.)}$$

which leads to our resulting Padé approximation:

$$Z(S) = \frac{1\sqrt{\pi} + (\pi - 2)S}{1 - i\sqrt{\pi}S - (\pi - 2)S^2} \qquad \text{(VI.16.)}$$

In Chapter 5 the values of the plasma function are required to compute the modified screening functions and in order to facilitate numerical calculations, rather than evaluate the integral expression (VI.1.), it is much faster to employ the algebraic approximation (VI.16.). The errors incurred by using this Padé approximation may be judged from Figure (VI.1.) which compares the real and imaginary parts of the plasma dispersion function for real argument determined from the exact integral form (VI.1.) against the approximation (VI.16.).

As can be seen, the approximation is a good representation of the plasma function thus justifying the use of a two-pole Padé approximant.



COMPARISON BETWEEN TABULATED VALUES OF FRIED & CONTE AND THE PADE APPROXIMATION (DOTTED LINE) TO THE PLASMA DISPERSION FUNCTION

Fig. VI.1.

The approximation (VI.16.) is the most accurate representation of the plasma function obtained to date as may be seen by comparing with other similar approximations[33][65].

APPENDIX VII

THE TWO-DIMENSIONAL MAXWELLIAN SCREENING FUNCTION

We repeat here the calculations of §5.2. to obtain a model screening function from the Lindhardt form (5.1.10.) appropriate to a 2-dimensional electron plasma with a Gaussian momentum distribution. The normalisation factor, $\exp(\beta\xi)$, is obtained by integrating to the total (areal) electron density, n, i.e.

$$n = \int dE\rho(E)f(E) \qquad \text{(VII.1.)}$$

where $\rho(E)$, the energy density of states in 2-dimensions is independent of energy since

$$\rho(E) = \frac{2}{(2\pi)^2} \times 2\pi k \frac{dk}{dE} \equiv \frac{m}{\hbar^2} \qquad \text{(VII.2.)}$$

Thus from (VII.1.) the normalisation factor is explicitly determined from

$$e^{\beta\xi} \equiv \frac{n\pi\hbar^2}{m\int_0^\infty e^{-\beta E}dE} \equiv \frac{n\pi\hbar^2}{m} \qquad \text{(VII.3.)}$$

Consequently from (5.1.10.) the appropriate screening function is:-

$$\begin{aligned}\epsilon[q,\omega] &= 1 + \frac{\phi(q)n\beta}{2\pi q}\int_0^\infty dk \int_0^{2\pi} d\theta k e^{-\lambda k^2}\left\{\frac{1}{k\cos\theta + \beta^+ + i\delta}\right. \\ &\qquad \left. + \frac{1}{k\cos\theta + \beta^- - i\delta}\right| \\ &= 1 + \frac{\theta(q)n\beta}{2\pi q\sqrt{\lambda}}\int_0^\infty dt t e^{-t^2}\int_0^{2\pi} d\theta\left\{\frac{1}{t\cos\theta + \alpha^+ + i\delta}\right. \\ &\qquad \left. + \frac{1}{t\cos\theta + \alpha^- - i\delta}\right| \end{aligned} \qquad \text{(VII.4.)}$$

where

$$\alpha^{\pm} = \sqrt{\lambda}\left[\frac{a}{2} \pm \frac{m\omega}{\hbar q}\right] \tag{VII.5.}$$

It is convenient to consider the real and imaginary parts of (VII.4.) separately. First, the imaginary part:

$$\begin{aligned}\mathrm{Im}\epsilon[q,\omega] &= \frac{-n\beta\phi(q)}{2q\sqrt{\lambda}} \int_0^{\infty} dt\, te^{-t^2} \int_0^{2\pi} d\theta \{\delta[t\cos\theta + \alpha^+] - \delta[t\cos\theta + \alpha^-]\} \\ &= \frac{-n\beta\phi(q)}{2q\sqrt{\lambda}} \int_0^{\infty} dt\, te^{-t^2} \int_0^{2\pi} d\theta \int_{-\infty}^{\infty} \frac{d\eta}{2\pi} \left[e^{i\eta[t\cos\theta+\alpha^+]}\right. \\ &\quad \left. - e^{i\eta\, t\cos\theta+\alpha^-}\right] \end{aligned} \tag{VII.6.}$$

However we note that

$$\int_{-\infty}^{\infty} d\eta \int_0^{2\pi} d\eta e^{i\eta(t\cos\theta+\alpha)} = 2\pi \int_{-\infty}^{\infty} d\eta e^{i\eta\alpha} J_0(t\eta) \tag{VII.7.}$$

where J_0 is a zero-th order Bessel function[2]. Recasting (VII.7.) into a standard integral form gives[2]

$$\begin{aligned} &4\pi \int_{-\infty}^{\infty} d\eta \cos(\eta\alpha) J_0(\alpha t) \\ &\equiv \begin{cases} 4\pi/\sqrt{t^2 - \alpha^2} \\ 0 \end{cases} \quad \text{if} \quad \begin{cases} 0 \le \alpha < t \\ t < \alpha \end{cases} \end{aligned} \tag{VII.8.}$$

Using (VII.8.) in (VII.6.) reduces the imaginary part of the 2-dimensional screening function to the form

$$\begin{aligned}\mathrm{Im}\epsilon[q,\omega] &= \frac{-n\beta\phi(q)}{q\sqrt{\pi}} \left[\int_{\alpha^+}^{\infty} \frac{dt\, te^{-t^2}}{\sqrt{t^2 - (\alpha^+)^2}} - \int_{\alpha^-}^{\infty} \frac{dt\, te^{-t^2}}{\sqrt{t^2 - (\alpha^-)^2}}\right] \\ &= \frac{-n\beta\phi(q)}{q\sqrt{\lambda}} \{[e^{-(\alpha^+)^2} - e^{-(\alpha^-)^2}] \int_{-\infty}^{\infty} dt\, e^{-t^2}\} \\ &= \frac{-n\beta\phi(q)\sqrt{\pi}}{2q\sqrt{\lambda}} \{e^{-(x - \frac{a}{2})^2} - e^{-(x + \frac{a}{2})^2}\} \end{aligned} \tag{VII.9.}$$

where (x,a) are the same dimensionless variables introduced in (5.2.9.) and (5.2.10.).

$$\alpha^{\pm} = \sqrt{\lambda}\left[\frac{a}{2} \pm \frac{m\omega}{\hbar q}\right] \tag{VII.5.}$$

It is convenient to consider the real and imaginary parts of (VII.4.) separately. First, the imaginary part:

$$\begin{aligned}\mathrm{Im}\epsilon[q,\omega] &= \frac{-n\beta\phi(q)}{2q\sqrt{\lambda}} \int_0^{\infty} dt\, t e^{-t^2} \int_0^{2\pi} d\theta \{\delta[t\cos\theta + \alpha^+] - \delta[t\cos\theta + \alpha^-]\} \\ &= \frac{-n\beta\phi(q)}{2q\sqrt{\lambda}} \int_0^{\infty} dt\, t e^{-t^2} \int_0^{2\pi} d\theta \int_{-\infty}^{\infty} \frac{d\eta}{2\pi} \left[e^{i\eta[t\cos\theta+\alpha^+]} \right. \\ &\left. - e^{i\eta\, t\cos\theta+\alpha^-}\right] \end{aligned} \tag{VII.6.}$$

However we note that

$$\int_{-\infty}^{\infty} d\eta \int_0^{2\pi} d\eta e^{i\eta(t\cos\theta+\alpha)} = 2\pi \int_{-\infty}^{\infty} d\eta e^{i\eta\alpha} J_0(t\eta) \tag{VII.7.}$$

where J_0 is a zero-th order Bessel function[2]. Recasting (VII.7.) into a standard integral form gives[2]

$$\begin{aligned} & 4\pi \int_{-\infty}^{\infty} d\eta \cos(\eta\alpha) J_0(\alpha t) \\ & \equiv \begin{cases} 4\pi/\sqrt{t^2 - \alpha^2} & \text{if } 0 \le \alpha < t \\ 0 & \text{if } t < \alpha \end{cases} \end{aligned} \tag{VII.8.}$$

Using (VII.8.) in (VII.6.) reduces the imaginary part of the 2-dimensional screening function to the form

$$\begin{aligned}\mathrm{Im}\epsilon[q,\omega] &= \frac{-n\beta\phi(q)}{q\sqrt{\pi}} \left[\int_{\alpha^+}^{\infty} \frac{dt\, t e^{-t^2}}{\sqrt{t^2 - (\alpha^+)^2}} - \int_{\alpha^-}^{\infty} \frac{dt\, t e^{-t^2}}{\sqrt{t^2 - (\alpha^-)^2}}\right] \\ &= \frac{-n\beta\phi(q)}{q\sqrt{\lambda}} \{[e^{-(\alpha^+)^2} - e^{-(\alpha^-)^2}] \int_{-\infty}^{\infty} dt e^{-t^2}\} \\ &= \frac{-n\beta\phi(q)\sqrt{\pi}}{2q\sqrt{\lambda}} \{e^{-(x - \frac{a}{2})^2} - e^{-(x + \frac{a}{2})^2}\} \end{aligned} \tag{VII.9.}$$

where (x,a) are the same dimensionless variables introduced in (5.2.9.) and (5.2.10.).

Similarly, the real part of the two-dimensional screening function is given by

$$\mathrm{Re}\epsilon[q,\omega] = \frac{n\beta\phi(q)}{2\pi q\sqrt{\lambda}} \int_0^\infty dt\, te^{-t^2}\, P \int_0^{2\pi} d\theta \left\{ \frac{1}{t\cos\theta + \alpha^+} + \frac{1}{t\cos\theta + \alpha^-} \right\} \qquad \text{(VII.10.)}$$

However we note that

$$\int_0^{2\pi} d\theta \left\{ \frac{1}{t\cos\theta + \alpha} \right\} = \int_0^{\pi} d\theta \left\{ \frac{1}{t\cos\theta + \alpha} - \frac{1}{t\cos\theta - \alpha} \right\}$$

$$= 2 \int_0^\infty d\tau \left\{ \frac{1}{(\alpha + t) + (\alpha - t)\tau^2} + \frac{1}{(\alpha - t) + (\alpha + t)\tau^2} \right\}$$

where $\tau = \tan\theta/2$. This is solved as

$$\begin{cases} 2\pi/\sqrt{\alpha^2 - t^2} \\ 0 \end{cases} \quad \text{for} \quad \begin{cases} \alpha > t \\ \alpha < t \end{cases} \qquad \text{(VII.11.)}$$

which, upon substituting back into (VII.10.), gives the real part of the screening function determined as:

$$\mathrm{Re}\epsilon[q,\omega] = 1 + \frac{n\beta\phi(q)}{q\sqrt{\lambda}} \int_0^1 d(\cos\theta) \{\alpha^+ e^{-(\alpha^+)^2[1-\cos^2\theta]} + \alpha^- e^{-(\alpha^-)^2[1-\cos^2\theta]}\}$$

$$= 1 + \frac{n\beta\phi(q)}{q\sqrt{\lambda}} \{e^{-(\alpha^+)^2} \int_0^{\alpha^+} dt\, e^{t^2} + e^{-(\alpha^-)^2} \int_0^{\alpha^-} dt\, e^{t^2}\}$$

$$\equiv 1 + \frac{n\beta\phi(q)}{q\sqrt{\lambda}} \left\{ \frac{\mathrm{ReZ}(x - \frac{a}{2}) - \mathrm{ReZ}(x + \frac{a}{2})}{2} \right\} \qquad \text{(VII.12.)}$$

where we have employed the definition (VI.7.).

To reduce the screening function represented by (VII.9.) and (VII.12.) further, we need the two-dimensional Fourier transform of the bare Coulomb potential $e^2/4\pi\epsilon_\infty r$ given by

$$\phi(q) = \frac{e^2}{4\pi\epsilon_\infty}\int_0^\infty rdr\int_0^{2\pi} d\theta\ \frac{e^{iqr\cos\theta}}{r}$$

$$= \frac{e^2}{4\pi\epsilon_\infty}\int_0^\infty dr 2\pi J_0(qr)$$

$$= \frac{e^2}{2\epsilon_\infty q} \qquad \text{(VII.13.)}$$

where we have used the definition of the zeroth order Bessel function and the property[2] $\int_0^\infty dx J_0(x) = 1$.

Therefore the resulting 2-dimensional screening function is given by:-

$$\epsilon[q,\omega] = 1 + \left(\frac{\kappa_{2D}}{q}\right)\frac{[Z(x-\frac{a}{2}) - Z(x+\frac{a}{2})]}{2a} \qquad \text{(VII.14.)}$$

where as in Chapter 5, x is the ratio of electron phase to thermal velocity and "a" represents the ratio of thermal to kinetic wavelengths.

We have also introduced the definition of a two-dimensional screening length, $1/\kappa_{2D}$, where

$$\kappa_{2D} = \frac{ne^2\beta}{2\epsilon_\infty} \qquad \text{(VII.15.)}$$

(Compare with the 3-dimensional counterpart, $\kappa_{3D}^2 = ne^2\beta/\epsilon_\infty$).

The expression (VII.14.) is exploited in §5.5.

APPENDIX VIII

THE 3-DIMENSIONAL SCREENING FUNCTION INCLUDING CONSTANT COLLISIONAL DAMPING FOR A DISPLACED MAXWELLIAN DISTRIBUTION

From the basic definition of the screening function (5.1.2.) we have

$$\epsilon[q,\omega] = 1 - \phi(P) \int \frac{d\omega'}{2\pi} \frac{d\omega''}{2\pi} dP' \left[\frac{f(P' - P/2) - f(P' + P/2)}{\omega - \omega' + \omega''}\right] a(\omega', P' + \frac{P}{2}) a(\omega'', P' - \frac{P}{2}) \qquad \text{(VIII.1.)}$$

where, for constant collisional damping Γ the spectral function (5.1.3.) may be expressed as

$$a(P,\omega) = \frac{\Gamma + \delta}{[\omega - \epsilon(P)]^2 + \left(\frac{\Gamma + \delta}{2}\right)^2} \equiv \frac{1}{i}\left[\frac{1}{\omega - \epsilon(P) - \frac{i\Gamma}{2} - i\delta} - \frac{1}{\omega - \epsilon(P) + \frac{i\Gamma}{2} + i\delta}\right] \qquad \text{(VIII.2.)}$$

The frequency integrals in (VIII.1.) may be performed by complex analysis since the poles are explicit in the spectral function (VIII.2.). Therefore if we choose to close the complex ω' contour in the lower-half-plane then the relevant poles are at $\omega' = \epsilon(P') - i\Gamma/2 - i\delta$ and at $\omega' = \omega + \omega''$. However if we also choose the ω'' contour to close in the upper-half-plane then the only contributing pole corresponding to the ω'' integral will be $\epsilon(P'') + i\Gamma/2 + i\delta$.

Consequently using these poles in (VIII.1.), the screening function may be evaluated as:-

$$\epsilon[q,\omega] = 1 - \phi(P) \int dP' \int \frac{d\omega'}{2\pi i} \int \frac{d\omega''}{2\pi i} [f(P' - P/2) - f(P' + P/2)] \times \left[\frac{1}{\omega - \omega' + \omega''}\right]\left[\frac{1}{\omega' - \epsilon(+) + \frac{i\Gamma}{2} + i\delta}\right]\left[\frac{1}{\epsilon(-) + \frac{i\Gamma}{2} + i\delta - \omega''}\right]$$

$$\equiv 1 - \phi(P) \int dP' \frac{[f(P' + P/2) - f(P' - P/2)]}{\epsilon(P' + P/2) - \epsilon(P' - P/2) - \omega - i\Gamma - i\delta} \qquad \text{(VIII.3.)}$$

which is of the same form as the screening function without constant

collisional damping (5.1.6.) except that we have had to replace ω by $\omega + i\Gamma$.

We will now evaluate this screening function with the use of the distribution function

$$f(k) = e^{-\beta[\varepsilon(k)-\xi]}\{1 + 2\lambda k\cdot k_d\} \qquad \text{(VIII.4.)}$$

which may be considered to be a special case of a displaced Maxwellian:

$$f(k) = e^{\beta\xi}e^{-\beta\xi(k-k_d)} \qquad \text{(VIII.5.)}$$

where (VIII.4.) assumes the displacing wavevector k_d is small, $\varepsilon(k) = \hbar^2k^2/2m$ and so $\lambda = \hbar^2\beta/2m$.

Also the normalisation factor, $\exp(\beta\xi)$, was obtained in Chapter 5 by integrating to the electron density which gave (5.2.4.)

$$e^{\beta\xi} = \frac{n\beta\sqrt{\beta}(2\pi\hbar)^3}{2\pi\sqrt{\pi}2m\sqrt{2m}}$$

We also assume that the displacing wavevector k_d is parallel to the wavevector q so that

$$\frac{k\cdot q}{|q|} \equiv \frac{k\cdot k_d}{|k_d|}$$

and since the displacing wavevector is parallel to the constant electric field, this means that E and q are also aligned in this approximation.

Consequently the screening function (VIII.3.) is now expressible in the form

$$\epsilon[q,\omega(E,\Gamma)] = 1 + \frac{\phi(q)4\pi e^{\beta\xi}}{(2\pi)^3}\int_0^\infty dk \int_{-1}^{1} dx k^2 e^{-\lambda k^2}\{1 + 2\lambda k k_d x\}$$

$$\times \left\{\frac{1}{\frac{\hbar^2kqx}{m} + \frac{\hbar^2q^2}{2m} + \hbar\omega + i\delta} + \frac{1}{\frac{\hbar^2kqx}{m} + \frac{\hbar^2q^2}{2m} - \hbar\omega - i\delta}\right\} \qquad \text{(VIII.5.)}$$

The integrals involved in (VIII.5.) may be split into two parts

corresponding to the two parts of the distribution function, $\exp(-\lambda k^2)$ and $2\lambda k k_d x \exp(-\lambda k^2)$. The first part gives precisely the contribution evaluated in §5.2. giving the result (5.2.12.)

$$1 + \left(\frac{\kappa_D}{q}\right)^2 \frac{[Z(x - \frac{a}{2}) - Z(x + \frac{a}{2})]}{2a} \qquad \text{(VIII.6.)}$$

where "a" is determined in (5.2.10.) and the x-variable is now a complex quantity:

$$x = \sqrt{\frac{\beta m}{2}} \frac{\omega(E,\Gamma)}{q}$$

$$\equiv \sqrt{\frac{\beta m}{2}} \sqrt{\frac{eE}{2qm}} + \frac{i\Gamma}{2} \sqrt{\frac{2m\beta}{\hbar^2 q^2}} \qquad \text{(VIII.7.)}$$

The second part involves the integrals:

$$\frac{m8\pi\lambda k_d e^2 \exp(\beta\xi)}{\epsilon_\infty (2\pi)^3 q^3 \hbar^2} \int_0^\infty dk \int_{-1}^{1} dx k^2 e^{-\lambda k^2} \left\{ \frac{x}{x + \frac{m\omega}{\hbar kq} + \frac{q}{2k} + i\delta} \right.$$

$$\left. x \; \frac{x}{x - \frac{m\omega}{\hbar kq} + \frac{q}{2k} + i\delta} \right)$$

which may be evaluated and reduced to the form

$$\frac{\kappa_D^2 k_d}{q^3} \{2 + x[Z(x + \frac{a}{2}) + Z(x - \frac{a}{2})]$$

$$+ \frac{a^2[Z(x + \frac{a}{2}) - Z(x - \frac{a}{2})]}{2a}\} \qquad \text{(VIII.8.)}$$

where we have made use of the definitions of $\exp(\beta\xi)$, the plasma-function (VI.1.), the dimensionless parameters "a" (5.2.10.) and "x" (VIII.7.) and the inverse Debye screening length κ_D determined from (5.2.13.).

Thus combining (VIII.8.) with (VIII.6.) gives the resulting form for a screening function determined using a displaced Maxwellian distribution which makes allowances for constant collisional damping and where the displacing wavevector is assumed to be small:

$$\epsilon[q,\omega] = \left(1 + \frac{2\kappa_D^2 k_d}{q^3}\right) + \left(\frac{\kappa_D^2 k_d}{q^3}\right) x[Z(x + \tfrac{a}{2}) - Z(x - \tfrac{a}{2})] + \left(\frac{\kappa_D}{q}\right)^2 \left(1 - \frac{k_d a^2}{q}\right) \frac{[Z(x - \frac{a}{2}) - Z(x + \frac{a}{2})]}{2a} \qquad \text{(VIII.9.)}$$

where x is a complex valued quantity involving the collisional damping (VIII.7.)

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